Supporting Information:

Bandgap Engineering through Nanoporosity in ZnO

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Calculated properties, cell parameters and fractional coordinates of all 105 considered structures. Structures 1-86 are 4CN-based structures. Structures 87-105 are wz-ZnO-NP structures. Both sets are ordered with respect to increasing V_{pore}. When V_{pore} is the same for two or more structures, they are ordered relative to increasing E_{rel}.

Str 1 (WZ)
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.00 eV
E_{rel}: 0.00 eV/ZnO
$Pore_{max}$: 0.18 nm
V_{pore}: 0 %
D_{pore}: 0
cell parameters
3.280 3.280 5.300 90.00 90.00 120.00
fractional coordinates
Zn 0.646 0.376 0.852
Zn 0.312 0.709 0.352
O 0.312 0.709 0.730
O 0.646 0.376 0.230

Str 2 (4H)
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: -0.09 eV
E_{rel}: 0.01 eV/ZnO
$Pore_{max}$: 0.18 nm
V_{pore}: 0 %
D_{pore}: 0
cell parameters
3.273 3.273 10.639 90.00 90.00 120.00
fractional coordinates
Zn 0.000 0.000 0.906
Zn 0.667 0.333 0.656
Zn 0.000 0.000 0.406
Zn 0.333 0.667 0.156
O 0.667 0.333 0.844
O 0.000 0.000 0.595
O 0.333 0.667 0.344
O 0.000 0.000 0.095

Str 3 (6H)
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: -0.12 eV
E_{rel}: 0.01 eV/ZnO

$Pore_{max}$: 0.18 nm
V_{pore}: 0 %
D_{pore}: 0
cell parameters
3.271 3.271 15.970 90.00 90.00 120.00
fractional coordinates
Zn 0.000 0.000 1.000
Zn 0.333 0.667 0.833
Zn 0.667 0.333 0.667
Zn 0.000 0.000 0.500
Zn 0.667 0.333 0.333
Zn 0.333 0.667 0.167
O 0.000 0.000 0.875
O 0.333 0.667 0.708
O 0.667 0.333 0.541
O 0.000 0.000 0.375
O 0.667 0.333 0.208
O 0.333 0.667 0.041

Str 4 (ZB)
$\Delta E_{gap}(PBE_{GW-fit})$: -0.17 eV
E_{rel}: 0.01 eV/ZnO
$Pore_{max}$: 0.18 nm
V_{pore}: 0 %
D_{pore}: 0
cell parameters
4.620 4.620 4.620 90.00 90.00 90.00
fractional coordinates
Zn 0.500 0.203 0.750
Zn 0.000 0.703 0.750
Zn 0.500 0.703 0.250
Zn 0.000 0.203 0.250
O 0.750 0.953 0.500
O 0.250 0.453 0.500
O 0.750 0.453 0.000
O 0.250 0.953 0.000

Str 5 (64_2_5204)[18]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.02 eV
E_{rel}: 0.04 eV/ZnO
$Pore_{max}$: 0.18 nm
V_{pore}: 0 %
D_{pore}: 0
cell parameters
5.377 13.149 5.699 89.99 89.98 90.02
fractional coordinates
Zn 0.670 0.190 0.920
Zn 0.798 0.690 0.920
Zn 0.674 0.435 0.917
Zn 0.794 0.935 0.917
Zn 0.294 0.935 0.591
Zn 0.174 0.435 0.591

Zn 0.298 0.690 0.589
Zn 0.170 0.190 0.588
Zn 0.670 0.314 0.420
Zn 0.798 0.814 0.420
Zn 0.674 0.068 0.417
Zn 0.794 0.568 0.417
Zn 0.174 0.069 0.091
Zn 0.294 0.569 0.091
Zn 0.298 0.814 0.089
Zn 0.170 0.314 0.088
O 0.172 0.690 0.919
O 0.296 0.190 0.919
O 0.176 0.936 0.918
O 0.292 0.436 0.918
O 0.792 0.436 0.591
O 0.676 0.936 0.591
O 0.672 0.690 0.589
O 0.796 0.190 0.589
O 0.172 0.814 0.419
O 0.296 0.314 0.419
O 0.292 0.068 0.418
O 0.176 0.568 0.418
O 0.792 0.068 0.091
O 0.676 0.568 0.091
O 0.796 0.314 0.089
O 0.672 0.814 0.089

Str 6 (BYL)[19]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.05 eV
E_{rel}: 0.05 eV/ZnO
$Pore_{max}$: 0.18 nm
V_{pore}: 0 %
D_{pore}: 0
cell parameters
9.858 10.831 5.707 90.00 90.02 90.00
fractional coordinates
Zn 0.845 0.653 0.840
Zn 0.845 0.153 0.840
Zn 0.169 0.653 0.839
Zn 0.169 0.153 0.839
Zn 0.507 0.589 0.836
Zn 0.507 0.089 0.836
Zn 0.007 0.905 0.666
Zn 0.007 0.405 0.666
Zn 0.669 0.841 0.663
Zn 0.669 0.341 0.663
Zn 0.346 0.841 0.662
Zn 0.346 0.341 0.662
Zn 0.346 0.591 0.339
Zn 0.346 0.091 0.339
Zn 0.669 0.591 0.339
Zn 0.669 0.091 0.339

Zn 0.007 0.655 0.336
Zn 0.007 0.155 0.336
Zn 0.507 0.839 0.166
Zn 0.507 0.339 0.166
Zn 0.169 0.903 0.163
Zn 0.169 0.403 0.163
Zn 0.845 0.903 0.163
Zn 0.845 0.403 0.163
O 0.845 0.843 0.837
O 0.845 0.343 0.837
O 0.170 0.843 0.837
O 0.169 0.343 0.837
O 0.507 0.903 0.837
O 0.507 0.403 0.837
O 0.007 0.591 0.665
O 0.007 0.091 0.665
O 0.669 0.651 0.664
O 0.669 0.151 0.664
O 0.345 0.651 0.664
O 0.345 0.151 0.664
O 0.669 0.901 0.338
O 0.669 0.401 0.338
O 0.345 0.901 0.338
O 0.345 0.401 0.338
O 0.007 0.341 0.337
O 0.007 0.841 0.337
O 0.507 0.653 0.165
O 0.507 0.153 0.165
O 0.845 0.593 0.165
O 0.845 0.093 0.165
O 0.169 0.593 0.165
O 0.169 0.093 0.165

Str 7 (64_2_7625)[18]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.07 eV
E_{rel}: 0.05 eV/ZnO
$Pore_{max}$: 0.17 nm
V_{pore}: 0 %
D_{pore}: 0
cell parameters
5.585 6.513 11.371 90.00 90.01 89.99
fractional coordinates
Zn 0.304 0.321 0.924
Zn 0.167 0.821 0.924
Zn 0.667 0.049 0.833
Zn 0.804 0.549 0.833
Zn 0.304 0.549 0.673
Zn 0.167 0.049 0.673
Zn 0.667 0.821 0.583
Zn 0.804 0.321 0.583
Zn 0.167 0.795 0.424
Zn 0.304 0.295 0.424

Zn 0.804 0.066 0.333
Zn 0.667 0.567 0.333
Zn 0.167 0.566 0.173
Zn 0.304 0.066 0.173
Zn 0.667 0.795 0.083
Zn 0.804 0.295 0.083
O 0.801 0.817 0.923
O 0.670 0.317 0.923
O 0.301 0.052 0.833
O 0.170 0.552 0.833
O 0.670 0.552 0.673
O 0.801 0.052 0.673
O 0.301 0.818 0.583
O 0.170 0.318 0.583
O 0.802 0.798 0.423
O 0.670 0.298 0.423
O 0.301 0.564 0.333
O 0.170 0.064 0.333
O 0.801 0.564 0.173
O 0.670 0.064 0.173
O 0.301 0.798 0.083
O 0.170 0.298 0.083

Str 8
$\Delta E_{gap}(PBE_{GW-fit})$: 0.07 eV
E_{rel}: 0.05 eV/ZnO
$Pore_{max}$: 0.17 nm
V_{pore}: 0 %
D_{pore}: 0
cell parameters
6.516 19.702 5.578 90.00 90.00 60.06
fractional coordinates
Zn 0.660 0.058 0.729
Zn 0.160 0.558 0.728
Zn 0.666 0.224 0.728
Zn 0.166 0.724 0.728
Zn 0.644 0.391 0.728
Zn 0.144 0.891 0.728
Zn 0.144 0.391 0.593
Zn 0.644 0.891 0.593
Zn 0.166 0.224 0.593
Zn 0.666 0.724 0.593
Zn 0.160 0.058 0.593
Zn 0.660 0.558 0.593
Zn 0.805 0.285 0.229
Zn 0.305 0.785 0.228
Zn 0.799 0.118 0.228
Zn 0.299 0.618 0.228
Zn 0.322 0.451 0.228
Zn 0.822 0.951 0.228
Zn 0.822 0.451 0.093
Zn 0.322 0.951 0.093

Zn 0.299 0.118 0.093
Zn 0.799 0.618 0.093
Zn 0.305 0.285 0.093
Zn 0.805 0.785 0.093
O 0.306 0.285 0.726
O 0.302 0.118 0.726
O 0.802 0.618 0.726
O 0.806 0.785 0.726
O 0.820 0.451 0.726
O 0.320 0.951 0.726
O 0.320 0.452 0.595
O 0.820 0.951 0.595
O 0.806 0.285 0.595
O 0.802 0.118 0.595
O 0.302 0.618 0.594
O 0.306 0.785 0.594
O 0.164 0.224 0.227
O 0.664 0.724 0.227
O 0.159 0.058 0.226
O 0.659 0.558 0.226
O 0.146 0.391 0.226
O 0.646 0.891 0.226
O 0.646 0.391 0.095
O 0.659 0.058 0.095
O 0.146 0.891 0.095
O 0.159 0.558 0.095
O 0.663 0.225 0.094
O 0.163 0.725 0.094

Str 9 (64_1_1)[18]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.08 eV
E_{rel}: 0.06 eV/ZnO
$Pore_{max}$: 0.17 nm
V_{pore}: 0 %
D_{pore}: 0
cell parameters
5.706 6.513 5.566 90.00 90.00 90.00
fractional coordinates
Zn 0.555 0.813 0.715
Zn 0.055 0.045 0.715
Zn 0.555 0.313 0.582
Zn 0.055 0.545 0.582
Zn 0.875 0.813 0.215
Zn 0.375 0.045 0.215
Zn 0.875 0.313 0.082
Zn 0.375 0.545 0.082
O 0.874 0.312 0.714
O 0.374 0.546 0.714
O 0.874 0.812 0.582
O 0.374 0.046 0.582
O 0.055 0.546 0.214
O 0.555 0.312 0.214

O 0.055 0.046 0.082
O 0.555 0.812 0.082

Str 10 (59_4_253337)[18]
$\Delta E_{gap}(PBE_{GW-fit})$: -0.01 eV
E_{rel}: 0.02 eV/ZnO
$Pore_{max}$: 0.18 nm
V_{pore}: 1 %
D_{pore}: 1
cell parameters
22.770 5.328 6.577 90.00 90.00 90.00
fractional coordinates
Zn 0.669 0.175 0.754
Zn 0.834 0.675 0.754
Zn 0.334 0.806 0.754
Zn 0.169 0.306 0.754
Zn 0.918 0.177 0.754
Zn 0.585 0.677 0.754
Zn 0.418 0.305 0.754
Zn 0.085 0.805 0.754
Zn 0.793 0.177 0.504
Zn 0.957 0.680 0.504
Zn 0.710 0.677 0.504
Zn 0.457 0.801 0.504
Zn 0.046 0.301 0.504
Zn 0.546 0.180 0.504
Zn 0.293 0.305 0.504
Zn 0.210 0.805 0.504
Zn 0.669 0.175 0.254
Zn 0.169 0.306 0.254
Zn 0.918 0.177 0.254
Zn 0.834 0.675 0.254
Zn 0.334 0.806 0.254
Zn 0.585 0.677 0.254
Zn 0.418 0.305 0.254
Zn 0.085 0.805 0.254
Zn 0.957 0.680 0.004
Zn 0.793 0.177 0.004
Zn 0.710 0.677 0.004
Zn 0.457 0.801 0.004
Zn 0.046 0.301 0.004
Zn 0.293 0.305 0.004
Zn 0.210 0.805 0.004
Zn 0.546 0.180 0.004
O 0.586 0.299 0.754
O 0.335 0.183 0.754
O 0.169 0.683 0.754
O 0.917 0.799 0.754
O 0.835 0.299 0.754
O 0.669 0.799 0.754
O 0.417 0.682 0.754
O 0.086 0.182 0.754

O 0.545 0.795 0.504
O 0.710 0.299 0.504
O 0.458 0.187 0.504
O 0.293 0.683 0.504
O 0.210 0.182 0.504
O 0.793 0.799 0.504
O 0.958 0.294 0.504
O 0.045 0.687 0.504
O 0.586 0.299 0.254
O 0.335 0.183 0.254
O 0.169 0.683 0.254
O 0.917 0.799 0.254
O 0.835 0.299 0.254
O 0.669 0.799 0.254
O 0.417 0.682 0.254
O 0.086 0.182 0.254
O 0.545 0.795 0.004
O 0.710 0.299 0.004
O 0.458 0.187 0.004
O 0.293 0.683 0.004
O 0.210 0.182 0.004
O 0.793 0.799 0.004
O 0.958 0.294 0.004
O 0.045 0.687 0.004

Str 11 (59_3_250)[18]
$\Delta E_{gap}(PBE_{GW-fit})$: -0.01 eV
E_{rel}: 0.02 eV/ZnO
$Pore_{max}$: 0.18 nm
V_{pore}: 1 %
D_{pore}: 1
cell parameters
17.069 5.342 3.288 90.00 90.00 90.00
fractional coordinates
Zn 0.443 0.793 0.771
Zn 0.114 0.797 0.770
Zn 0.226 0.300 0.770
Zn 0.891 0.167 0.770
Zn 0.779 0.665 0.770
Zn 0.561 0.172 0.770
Zn 0.279 0.800 0.271
Zn 0.391 0.298 0.271
Zn 0.943 0.672 0.270
Zn 0.061 0.292 0.270
Zn 0.614 0.668 0.270
Zn 0.725 0.165 0.270
O 0.225 0.676 0.771
O 0.444 0.178 0.771
O 0.890 0.791 0.770
O 0.114 0.173 0.770
O 0.561 0.787 0.770
O 0.780 0.289 0.770

O 0.390 0.674 0.271
O 0.061 0.677 0.270
O 0.280 0.176 0.270
O 0.944 0.287 0.270
O 0.725 0.789 0.270
O 0.614 0.291 0.270

Str 12 (59_4_280312)[18]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.00 eV
E_{rel}: 0.03 eV/ZnO
$Pore_{max}$: 0.18 nm
V_{pore}: 1 %
D_{pore}: 1
cell parameters
11.372 5.375 6.586 90.00 90.00 90.00
fractional coordinates
Zn 0.835 0.322 0.750
Zn 0.665 0.822 0.750
Zn 0.335 0.189 0.750
Zn 0.165 0.689 0.750
Zn 0.911 0.818 0.500
Zn 0.589 0.318 0.500
Zn 0.411 0.694 0.500
Zn 0.089 0.194 0.500
Zn 0.835 0.322 0.250
Zn 0.665 0.822 0.250
Zn 0.335 0.189 0.250
Zn 0.165 0.689 0.250
Zn 0.911 0.818 0.000
Zn 0.589 0.318 0.000
Zn 0.411 0.694 0.000
Zn 0.089 0.194 0.000
O 0.833 0.696 0.750
O 0.668 0.196 0.750
O 0.333 0.815 0.750
O 0.168 0.315 0.750
O 0.913 0.200 0.500
O 0.587 0.700 0.500
O 0.413 0.311 0.500
O 0.087 0.811 0.500
O 0.833 0.696 0.250
O 0.668 0.196 0.250
O 0.333 0.815 0.250
O 0.168 0.315 0.250
O 0.913 0.200 0.000
O 0.587 0.700 0.000
O 0.413 0.311 0.000
O 0.087 0.811 0.000

Str 13
$\Delta E_{gap}(PBE_{GW-fit})$: 0.03 eV
E_{rel}: 0.06 eV/ZnO

$Pore_{max}$: 0.19 nm
V_{pore}: 2 %
D_{pore}: 1
cell parameters
6.601 13.178 5.389 89.86 90.00 59.94
fractional coordinates
Zn 0.149 0.591 0.726
Zn 0.148 0.841 0.725
Zn 0.649 0.841 0.725
Zn 0.653 0.586 0.606
Zn 0.644 0.096 0.599
Zn 0.145 0.338 0.599
Zn 0.659 0.338 0.599
Zn 0.146 0.094 0.598
Zn 0.819 0.920 0.223
Zn 0.306 0.676 0.222
Zn 0.820 0.677 0.222
Zn 0.322 0.918 0.222
Zn 0.312 0.428 0.215
Zn 0.316 0.173 0.096
Zn 0.817 0.173 0.096
Zn 0.816 0.424 0.095
O 0.316 0.173 0.721
O 0.818 0.173 0.721
O 0.817 0.422 0.721
O 0.313 0.427 0.614
O 0.820 0.676 0.605
O 0.307 0.676 0.605
O 0.819 0.921 0.605
O 0.321 0.919 0.604
O 0.644 0.096 0.217
O 0.146 0.093 0.216
O 0.145 0.338 0.216
O 0.658 0.338 0.216
O 0.652 0.587 0.208
O 0.148 0.592 0.100
O 0.650 0.841 0.100
O 0.148 0.841 0.100

Str 14 (59_4_253313)[18]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.00 eV
E_{rel}: 0.05 eV/ZnO
$Pore_{max}$: 0.18 nm
V_{pore}: 2 %
D_{pore}: 1
cell parameters
22.669 5.462 6.584 90.02 89.99 89.99
fractional coordinates
Zn 0.078 0.683 0.752
Zn 0.417 0.183 0.752
Zn 0.578 0.812 0.752
Zn 0.917 0.312 0.752

Zn 0.668 0.185 0.752
Zn 0.327 0.811 0.752
Zn 0.168 0.311 0.752
Zn 0.827 0.684 0.752
Zn 0.452 0.682 0.502
Zn 0.042 0.182 0.502
Zn 0.290 0.313 0.502
Zn 0.952 0.813 0.502
Zn 0.790 0.182 0.502
Zn 0.705 0.682 0.502
Zn 0.205 0.813 0.502
Zn 0.543 0.313 0.502
Zn 0.078 0.683 0.252
Zn 0.417 0.183 0.252
Zn 0.917 0.312 0.252
Zn 0.578 0.812 0.252
Zn 0.668 0.185 0.252
Zn 0.327 0.811 0.252
Zn 0.168 0.311 0.252
Zn 0.827 0.684 0.252
Zn 0.452 0.682 0.002
Zn 0.042 0.182 0.002
Zn 0.290 0.313 0.002
Zn 0.205 0.813 0.002
Zn 0.952 0.813 0.002
Zn 0.790 0.182 0.002
Zn 0.705 0.682 0.002
Zn 0.543 0.313 0.002
O 0.416 0.809 0.752
O 0.079 0.308 0.752
O 0.667 0.810 0.752
O 0.828 0.309 0.752
O 0.916 0.687 0.752
O 0.328 0.186 0.752
O 0.167 0.686 0.752
O 0.579 0.187 0.752
O 0.042 0.808 0.502
O 0.453 0.309 0.502
O 0.542 0.687 0.502
O 0.953 0.186 0.502
O 0.706 0.313 0.502
O 0.289 0.682 0.502
O 0.789 0.813 0.502
O 0.206 0.182 0.502
O 0.416 0.809 0.252
O 0.079 0.308 0.252
O 0.828 0.309 0.252
O 0.667 0.810 0.252
O 0.916 0.687 0.252
O 0.328 0.186 0.252
O 0.167 0.686 0.252
O 0.579 0.187 0.252

O 0.042 0.808 0.002
O 0.453 0.309 0.002
O 0.542 0.687 0.002
O 0.953 0.186 0.002
O 0.706 0.313 0.002
O 0.289 0.682 0.002
O 0.789 0.813 0.002
O 0.206 0.182 0.002

Str 15
$\Delta E_{gap}(PBE_{GW-fit})$: 0.06 eV
E_{rel}: 0.08 eV/ZnO
$Pore_{max}$: 0.19 nm
V_{pore}: 2 %
D_{pore}: 1
cell parameters
9.962 9.921 5.371 89.63 90.00 120.14
fractional coordinates
Zn 0.895 0.441 0.817
Zn 0.561 0.441 0.817
Zn 0.228 0.441 0.817
Zn 0.558 0.101 0.703
Zn 0.891 0.101 0.702
Zn 0.224 0.101 0.702
Zn 0.896 0.778 0.690
Zn 0.563 0.778 0.690
Zn 0.230 0.778 0.690
Zn 0.780 0.545 0.315
Zn 0.446 0.545 0.315
Zn 0.113 0.545 0.315
Zn 0.785 0.222 0.302
Zn 0.452 0.222 0.302
Zn 0.118 0.222 0.302
Zn 0.782 0.882 0.188
Zn 0.115 0.882 0.188
Zn 0.448 0.882 0.188
O 0.781 0.881 0.811
O 0.114 0.881 0.811
O 0.448 0.881 0.811
O 0.785 0.221 0.709
O 0.451 0.221 0.709
O 0.118 0.222 0.709
O 0.780 0.545 0.698
O 0.447 0.545 0.698
O 0.113 0.545 0.698
O 0.896 0.778 0.307
O 0.563 0.778 0.307
O 0.230 0.778 0.307
O 0.558 0.101 0.297
O 0.891 0.102 0.296
O 0.225 0.102 0.296
O 0.895 0.442 0.194

O 0.562 0.442 0.194
O 0.228 0.442 0.193

Str 16 (189_3_1615)[18]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.07 eV
E_{rel}: 0.08 eV/ZnO
$Pore_{max}$: 0.23 nm
V_{pore}: 2 %
D_{pore}: 1
cell parameters
9.924 9.925 5.395 90.00 90.00 120.00
fractional coordinates
Zn 0.888 0.437 0.817
Zn 0.563 0.437 0.817
Zn 0.563 0.111 0.817
Zn 0.890 0.766 0.805
Zn 0.890 0.109 0.805
Zn 0.233 0.109 0.805
Zn 0.558 0.771 0.689
Zn 0.228 0.771 0.689
Zn 0.228 0.442 0.689
Zn 0.781 0.548 0.319
Zn 0.781 0.218 0.319
Zn 0.452 0.218 0.319
Zn 0.776 0.881 0.203
Zn 0.119 0.881 0.203
Zn 0.119 0.223 0.203
Zn 0.446 0.878 0.192
Zn 0.446 0.553 0.192
Zn 0.121 0.553 0.192
O 0.447 0.879 0.811
O 0.447 0.553 0.811
O 0.121 0.553 0.811
O 0.119 0.881 0.800
O 0.119 0.223 0.800
O 0.776 0.881 0.800
O 0.781 0.548 0.694
O 0.781 0.218 0.694
O 0.452 0.218 0.694
O 0.558 0.771 0.315
O 0.228 0.771 0.315
O 0.228 0.442 0.315
O 0.890 0.766 0.208
O 0.890 0.109 0.208
O 0.233 0.109 0.208
O 0.563 0.437 0.198
O 0.889 0.437 0.198
O 0.563 0.111 0.198

Str 17
$\Delta E_{gap}(PBE_{GW-fit})$: 0.04 eV
E_{rel}: 0.08 eV/ZnO

$Pore_{max}$: 0.19 nm

V_{pore}: 2 %

D_{pore}: 1

cell parameters

22.823 5.416 6.631 90.02 89.99 90.33

fractional coordinates

Zn 0.422 0.303 0.754
Zn 0.582 0.679 0.754
Zn 0.837 0.696 0.754
Zn 0.332 0.674 0.754
Zn 0.919 0.181 0.754
Zn 0.084 0.814 0.754
Zn 0.671 0.311 0.754
Zn 0.167 0.297 0.754
Zn 0.547 0.176 0.505
Zn 0.294 0.177 0.504
Zn 0.212 0.694 0.504
Zn 0.791 0.297 0.504
Zn 0.958 0.683 0.504
Zn 0.046 0.312 0.504
Zn 0.709 0.811 0.504
Zn 0.457 0.805 0.504
Zn 0.422 0.303 0.255
Zn 0.582 0.679 0.254
Zn 0.837 0.696 0.254
Zn 0.332 0.674 0.254
Zn 0.919 0.181 0.254
Zn 0.084 0.814 0.254
Zn 0.671 0.311 0.254
Zn 0.167 0.297 0.254
Zn 0.547 0.176 0.005
Zn 0.294 0.177 0.004
Zn 0.212 0.694 0.004
Zn 0.958 0.683 0.004
Zn 0.791 0.297 0.004
Zn 0.046 0.312 0.004
Zn 0.709 0.811 0.004
Zn 0.457 0.805 0.004
O 0.583 0.300 0.755
O 0.333 0.297 0.754
O 0.167 0.701 0.754
O 0.919 0.807 0.754
O 0.837 0.292 0.754
O 0.084 0.187 0.754
O 0.421 0.682 0.754
O 0.670 0.688 0.754
O 0.545 0.799 0.505
O 0.458 0.183 0.504
O 0.791 0.701 0.504
O 0.295 0.802 0.504
O 0.958 0.304 0.504
O 0.045 0.692 0.504

O 0.709 0.185 0.504
O 0.212 0.291 0.504
O 0.583 0.300 0.255
O 0.333 0.297 0.254
O 0.167 0.701 0.254
O 0.919 0.807 0.254
O 0.837 0.292 0.254
O 0.084 0.187 0.254
O 0.421 0.682 0.254
O 0.670 0.688 0.254
O 0.545 0.799 0.005
O 0.458 0.183 0.004
O 0.791 0.701 0.004
O 0.295 0.802 0.004
O 0.958 0.304 0.004
O 0.045 0.692 0.004
O 0.709 0.185 0.004
O 0.212 0.291 0.004

Str 18 (SSCCCC)[16]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.08 eV
E_{rel}: 0.09 eV/ZnO
$Pore_{max}$: 0.19 nm
V_{pore}: 3 %
D_{pore}: 0
cell parameters
11.462 5.320 3.331 89.99 90.00 90.00
fractional coordinates
Zn 0.278 0.187 0.920
Zn 0.615 0.804 0.919
Zn 0.778 0.285 0.919
Zn 0.115 0.667 0.919
Zn 0.370 0.785 0.420
Zn 0.533 0.304 0.420
Zn 0.033 0.168 0.419
Zn 0.870 0.687 0.419
O 0.279 0.778 0.920
O 0.613 0.183 0.919
O 0.114 0.289 0.919
O 0.779 0.694 0.919
O 0.369 0.193 0.419
O 0.535 0.683 0.419
O 0.869 0.278 0.419
O 0.035 0.789 0.419

Str 19
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.11 eV
E_{rel}: 0.10 eV/ZnO
$Pore_{max}$: 0.23 nm
V_{pore}: 3 %
D_{pore}: 1
cell parameters

8.769 6.624 5.461 89.98 90.03 79.20
fractional coordinates
Zn 0.556 0.617 0.996
Zn 0.889 0.294 0.994
Zn 0.560 0.116 0.873
Zn 0.217 0.943 0.873
Zn 0.218 0.457 0.872
Zn 0.889 0.792 0.861
Zn 0.773 0.553 0.495
Zn 0.444 0.887 0.482
Zn 0.102 0.228 0.481
Zn 0.445 0.401 0.481
Zn 0.773 0.050 0.361
Zn 0.106 0.727 0.359
O 0.106 0.727 0.988
O 0.775 0.055 0.986
O 0.445 0.401 0.879
O 0.445 0.887 0.878
O 0.103 0.229 0.878
O 0.773 0.557 0.870
O 0.889 0.787 0.486
O 0.559 0.116 0.476
O 0.217 0.457 0.475
O 0.217 0.943 0.475
O 0.887 0.290 0.369
O 0.556 0.617 0.366

Str 20
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.13 eV
E_{rel}: 0.13 eV/ZnO
$Pore_{max}$: 0.22 nm
V_{pore}: 3 %
D_{pore}: 1
cell parameters
6.671 6.671 5.373 90.00 90.00 120.00
fractional coordinates
Zn 0.825 0.648 0.961
Zn 0.825 0.158 0.961
Zn 0.335 0.158 0.961
Zn 0.655 0.818 0.562
Zn 0.165 0.818 0.562
Zn 0.165 0.328 0.562
Zn 0.662 0.321 0.446
Zn 0.329 0.655 0.077
O 0.655 0.818 0.967
O 0.166 0.818 0.967
O 0.166 0.329 0.967
O 0.825 0.647 0.555
O 0.825 0.158 0.555
O 0.336 0.158 0.555
O 0.329 0.655 0.454
O 0.662 0.321 0.068

Str 21 (BCT)[17]
ΔE_{gap}(PBE$_{GW-fit}$): 0.03 eV
E_{rel}: 0.05 eV/ZnO
Pore$_{max}$: 0.16 nm
V_{pore}: 3 %
D_{pore}: 1
cell parameters
7.925 7.925 3.287 90.00 90.00 90.00
fractional coordinates
Zn 0.503 0.818 0.500
Zn 0.503 0.182 0.500
Zn 0.003 0.682 0.500
Zn 0.003 0.318 0.500
Zn 0.821 0.000 0.000
Zn 0.685 0.500 0.000
Zn 0.321 0.500 0.000
Zn 0.185 0.000 0.000
O 0.821 0.500 0.500
O 0.685 0.000 0.500
O 0.321 0.000 0.500
O 0.185 0.500 0.500
O 0.503 0.682 0.000
O 0.503 0.318 0.000
O 0.003 0.818 0.000
O 0.003 0.182 0.000

Str 22
ΔE_{gap}(PBE$_{GW-fit}$): 0.07 eV
E_{rel}: 0.07 eV/ZnO
Pore$_{max}$: 0.19 nm
V_{pore}: 3 %
D_{pore}: 1
cell parameters
8.711 6.587 5.484 90.16 90.17 79.25
fractional coordinates
Zn 0.780 0.034 0.874
Zn 0.780 0.534 0.874
Zn 0.458 0.856 0.874
Zn 0.340 0.154 0.507
Zn 0.017 0.976 0.507
Zn 0.018 0.475 0.506
Zn 0.347 0.654 0.380
Zn 0.686 0.307 0.378
Zn 0.678 0.810 0.371
Zn 0.119 0.199 0.009
Zn 0.112 0.702 0.003
Zn 0.451 0.357 0.001
O 0.345 0.649 0.993
O 0.339 0.149 0.881
O 0.015 0.474 0.881
O 0.015 0.977 0.881

O 0.782 0.032 0.500
O 0.459 0.862 0.500
O 0.783 0.536 0.500
O 0.453 0.361 0.388
O 0.114 0.702 0.380
O 0.120 0.199 0.377
O 0.678 0.810 0.003
O 0.684 0.308 0.001

Str 23 (-LIT)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.12 eV
E_{rel}: 0.10 eV/ZnO
$Pore_{max}$: 0.20 nm
V_{pore}: 5 %
D_{pore}: 1
cell parameters
9.891 5.586 5.716 90.00 90.00 90.00
fractional coordinates
Zn 0.994 0.935 0.840
Zn 0.670 0.933 0.831
Zn 0.332 0.065 0.817
Zn 0.832 0.435 0.683
Zn 0.170 0.567 0.669
Zn 0.494 0.565 0.660
Zn 0.506 0.065 0.340
Zn 0.830 0.067 0.331
Zn 0.168 0.935 0.317
Zn 0.668 0.565 0.183
Zn 0.330 0.433 0.169
Zn 0.006 0.435 0.160
O 0.995 0.563 0.838
O 0.668 0.558 0.834
O 0.332 0.436 0.818
O 0.832 0.064 0.682
O 0.168 0.942 0.666
O 0.495 0.937 0.662
O 0.505 0.437 0.338
O 0.832 0.442 0.334
O 0.168 0.564 0.318
O 0.668 0.936 0.182
O 0.332 0.058 0.166
O 0.005 0.063 0.162

Str 24 (64_2_7619)[18]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.14 eV
E_{rel}: 0.11 eV/ZnO
$Pore_{max}$: 0.20 nm
V_{pore}: 5 %
D_{pore}: 2
cell parameters
5.630 6.563 11.501 90.00 90.00 90.00
fractional coordinates

Zn 0.803 0.003 0.914
Zn 0.673 0.503 0.914
Zn 0.307 0.231 0.830
Zn 0.169 0.731 0.830
Zn 0.807 0.231 0.669
Zn 0.669 0.731 0.669
Zn 0.303 0.003 0.586
Zn 0.173 0.503 0.586
Zn 0.803 0.489 0.414
Zn 0.673 0.989 0.414
Zn 0.307 0.260 0.330
Zn 0.169 0.760 0.330
Zn 0.807 0.260 0.169
Zn 0.669 0.760 0.169
Zn 0.303 0.489 0.086
Zn 0.173 0.989 0.086
O 0.296 0.497 0.915
O 0.180 0.997 0.915
O 0.803 0.735 0.829
O 0.674 0.235 0.829
O 0.303 0.735 0.671
O 0.174 0.235 0.671
O 0.796 0.497 0.585
O 0.680 0.997 0.585
O 0.296 0.994 0.415
O 0.180 0.494 0.415
O 0.803 0.757 0.329
O 0.674 0.257 0.329
O 0.303 0.757 0.171
O 0.174 0.257 0.171
O 0.796 0.994 0.085
O 0.680 0.494 0.085

Str 25 (64_2_5457)[18]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.18 eV
E_{rel}: 0.11 eV/ZnO
$Pore_{max}$: 0.20 nm
V_{pore}: 5 %
D_{pore}: 2
cell parameters
5.647 13.252 5.680 90.00 90.00 90.00
fractional coordinates
Zn 0.305 0.691 0.907
Zn 0.173 0.191 0.907
Zn 0.170 0.935 0.902
Zn 0.308 0.435 0.902
Zn 0.808 0.435 0.595
Zn 0.670 0.935 0.595
Zn 0.673 0.191 0.591
Zn 0.805 0.692 0.591
Zn 0.305 0.806 0.407
Zn 0.173 0.306 0.407

Zn 0.308 0.062 0.402
Zn 0.171 0.562 0.402
Zn 0.807 0.062 0.095
Zn 0.671 0.562 0.095
Zn 0.673 0.306 0.091
Zn 0.805 0.806 0.091
O 0.807 0.191 0.911
O 0.671 0.691 0.910
O 0.797 0.935 0.910
O 0.681 0.435 0.910
O 0.297 0.935 0.587
O 0.181 0.435 0.587
O 0.307 0.191 0.587
O 0.171 0.691 0.587
O 0.807 0.306 0.411
O 0.671 0.806 0.411
O 0.798 0.562 0.410
O 0.680 0.062 0.410
O 0.180 0.062 0.087
O 0.297 0.562 0.087
O 0.171 0.806 0.087
O 0.307 0.306 0.087

Str 26 (AEN)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.21 eV
E_{rel}: 0.12 eV/ZnO
$Pore_{max}$: 0.24 nm
V_{pore}: 5 %
D_{pore}: 1
cell parameters
6.690 8.692 10.869 90.00 90.01 90.00
fractional coordinates
Zn 0.872 0.509 0.938
Zn 0.372 0.509 0.938
Zn 0.622 0.821 0.836
Zn 0.122 0.821 0.836
Zn 0.622 0.197 0.836
Zn 0.122 0.197 0.836
Zn 0.872 0.697 0.645
Zn 0.372 0.697 0.645
Zn 0.872 0.321 0.645
Zn 0.372 0.321 0.645
Zn 0.622 0.009 0.544
Zn 0.122 0.009 0.544
Zn 0.622 0.509 0.438
Zn 0.122 0.509 0.438
Zn 0.872 0.197 0.336
Zn 0.372 0.197 0.336
Zn 0.872 0.821 0.336
Zn 0.372 0.821 0.336
Zn 0.622 0.321 0.145
Zn 0.122 0.321 0.145

Zn 0.622 0.697 0.145
Zn 0.122 0.697 0.145
Zn 0.872 0.009 0.044
Zn 0.372 0.009 0.044
O 0.622 0.009 0.936
O 0.122 0.009 0.936
O 0.872 0.697 0.837
O 0.872 0.321 0.837
O 0.372 0.697 0.837
O 0.372 0.321 0.837
O 0.122 0.821 0.644
O 0.622 0.821 0.644
O 0.622 0.197 0.644
O 0.122 0.197 0.644
O 0.872 0.509 0.545
O 0.372 0.509 0.545
O 0.872 0.009 0.436
O 0.372 0.009 0.436
O 0.622 0.321 0.337
O 0.122 0.321 0.337
O 0.622 0.697 0.337
O 0.122 0.697 0.337
O 0.872 0.197 0.144
O 0.372 0.197 0.144
O 0.872 0.821 0.144
O 0.372 0.821 0.144
O 0.622 0.509 0.045
O 0.122 0.509 0.045

Str 27 (ATV)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.20 eV
E_{rel}: 0.13 eV/ZnO
$Pore_{max}$: 0.23 nm
V_{pore}: 6 %
D_{pore}: 1
cell parameters
5.280 10.095 5.895 90.00 90.00 90.00
fractional coordinates
Zn 0.811 0.250 0.840
Zn 0.311 0.750 0.840
Zn 0.811 0.906 0.666
Zn 0.811 0.594 0.666
Zn 0.311 0.406 0.666
Zn 0.311 0.094 0.666
Zn 0.811 0.406 0.334
Zn 0.811 0.094 0.334
Zn 0.311 0.906 0.334
Zn 0.311 0.594 0.334
Zn 0.811 0.750 0.160
Zn 0.311 0.250 0.160
O 0.692 0.750 0.837
O 0.192 0.250 0.837

O 0.688 0.406 0.671
O 0.688 0.094 0.671
O 0.188 0.906 0.671
O 0.188 0.594 0.671
O 0.688 0.906 0.329
O 0.688 0.594 0.329
O 0.188 0.406 0.329
O 0.188 0.094 0.329
O 0.692 0.250 0.163
O 0.192 0.750 0.163

Str 28 (JBW)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.20 eV
E_{rel}: 0.19 eV/ZnO
$Pore_{max}$: 0.21 nm
V_{pore}: 7 %
D_{pore}: 1
cell parameters
3.353 10.166 4.751 90.00 90.00 90.00
fractional coordinates
Zn 0.750 0.608 0.893
Zn 0.750 0.904 0.893
Zn 0.750 0.256 0.610
Zn 0.250 0.756 0.389
Zn 0.250 0.405 0.106
Zn 0.250 0.108 0.106
O 0.750 0.408 0.871
O 0.750 0.104 0.871
O 0.750 0.756 0.626
O 0.250 0.256 0.374
O 0.250 0.604 0.128
O 0.250 0.908 0.128

Str 29 (SSCSSC)[16]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.31 eV
E_{rel}: 0.15 eV/ZnO
$Pore_{max}$: 0.22 nm
V_{pore}: 10 %
D_{pore}: 1
cell parameters
5.534 3.365 6.051 90.00 89.99 89.99
fractional coordinates
Zn 0.062 0.108 0.727
Zn 0.562 0.608 0.573
Zn 0.363 0.108 0.227
Zn 0.863 0.608 0.073
O 0.869 0.608 0.725
O 0.369 0.108 0.576
O 0.557 0.608 0.225
O 0.056 0.108 0.076

Str 30 (ABW)[17]

$\Delta E_{gap}(PBE_{GW-fit})$: 0.30 eV

E_{rel}: 0.15 eV/ZnO

$Pore_{max}$: 0.22 nm

V_{pore}: 10 %

D_{pore}: 1

cell parameters

12.188 6.707 11.061 90.00 90.00 90.00

fractional coordinates

Zn 0.912 0.500 0.998
Zn 0.912 0.000 0.998
Zn 0.412 0.500 0.998
Zn 0.412 0.000 0.998
Zn 0.585 0.750 0.899
Zn 0.585 0.250 0.899
Zn 0.085 0.750 0.899
Zn 0.085 0.250 0.899
Zn 0.835 0.750 0.748
Zn 0.835 0.250 0.748
Zn 0.335 0.750 0.748
Zn 0.335 0.250 0.748
Zn 0.662 0.500 0.649
Zn 0.662 0.000 0.649
Zn 0.162 0.500 0.649
Zn 0.162 0.000 0.649
Zn 0.912 0.500 0.498
Zn 0.912 0.000 0.498
Zn 0.412 0.500 0.498
Zn 0.412 0.000 0.498
Zn 0.585 0.750 0.399
Zn 0.585 0.250 0.399
Zn 0.085 0.750 0.399
Zn 0.085 0.250 0.399
Zn 0.835 0.750 0.248
Zn 0.835 0.250 0.248
Zn 0.335 0.750 0.248
Zn 0.335 0.250 0.248
Zn 0.662 0.500 0.149
Zn 0.662 0.000 0.149
Zn 0.162 0.500 0.149
Zn 0.162 0.000 0.149
O 0.585 0.500 0.997
O 0.585 0.000 0.997
O 0.085 0.500 0.997
O 0.085 0.000 0.997
O 0.912 0.750 0.900
O 0.912 0.250 0.900
O 0.412 0.750 0.900
O 0.412 0.250 0.900
O 0.662 0.750 0.747
O 0.662 0.250 0.747
O 0.162 0.750 0.747
O 0.162 0.250 0.747

O 0.835 0.500 0.650
O 0.835 0.000 0.650
O 0.335 0.500 0.650
O 0.335 0.000 0.650
O 0.585 0.500 0.497
O 0.585 0.000 0.497
O 0.085 0.500 0.497
O 0.085 0.000 0.497
O 0.912 0.750 0.400
O 0.912 0.250 0.400
O 0.412 0.750 0.400
O 0.412 0.250 0.400
O 0.662 0.750 0.247
O 0.662 0.250 0.247
O 0.162 0.750 0.247
O 0.162 0.250 0.247
O 0.835 0.500 0.150
O 0.835 0.000 0.150
O 0.335 0.500 0.150
O 0.335 0.000 0.150

Str 31 (DFT)[17]
ΔE_{gap}(PBE$_{GW-fit}$): 0.35 eV
E_{rel}: 0.14 eV/ZnO
Pore$_{max}$: 0.23 nm
V_{pore}: 10 %
D_{pore}: 1
cell parameters
8.631 8.631 8.907 57.08 122.92 96.99
fractional coordinates
Zn 0.710 0.449 0.862
Zn 0.210 0.949 0.862
Zn 0.818 0.840 0.862
Zn 0.318 0.340 0.862
Zn 0.715 0.795 0.521
Zn 0.323 0.686 0.521
Zn 0.823 0.186 0.521
Zn 0.215 0.295 0.521
Zn 0.494 0.516 0.362
Zn 0.994 0.016 0.362
Zn 0.885 0.624 0.362
Zn 0.385 0.124 0.362
Zn 0.539 0.619 0.021
Zn 0.039 0.119 0.021
Zn 0.648 0.011 0.021
Zn 0.148 0.511 0.021
O 0.883 0.624 0.865
O 0.383 0.124 0.865
O 0.997 0.011 0.865
O 0.496 0.511 0.865
O 0.536 0.624 0.519
O 0.036 0.124 0.519

O 0.649 0.011 0.519
O 0.149 0.511 0.519
O 0.823 0.837 0.365
O 0.323 0.337 0.365
O 0.709 0.450 0.365
O 0.209 0.951 0.365
O 0.824 0.184 0.019
O 0.324 0.684 0.019
O 0.710 0.797 0.019
O 0.210 0.297 0.019

Str 32 (SSSCSC)[16]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.36 eV
E_{rel}: 0.14 eV/ZnO
$Pore_{max}$: 0.23 nm
V_{pore}: 10 %
D_{pore}: 1
cell parameters
5.714 6.466 6.134 90.02 90.02 89.96
fractional coordinates
Zn 0.037 0.071 0.727
Zn 0.537 0.787 0.727
Zn 0.537 0.287 0.568
Zn 0.037 0.571 0.568
Zn 0.887 0.287 0.227
Zn 0.387 0.570 0.227
Zn 0.387 0.070 0.068
Zn 0.887 0.787 0.068
O 0.386 0.066 0.725
O 0.886 0.792 0.725
O 0.886 0.292 0.570
O 0.386 0.566 0.570
O 0.538 0.292 0.225
O 0.037 0.565 0.224
O 0.037 0.065 0.070
O 0.537 0.792 0.070

Str 33 (135_1_4)[18]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.32 eV
E_{rel}: 0.15 eV/ZnO
$Pore_{max}$: 0.28 nm
V_{pore}: 10 %
D_{pore}: 1
cell parameters
6.471 6.471 5.285 90.00 90.00 90.00
fractional coordinates
Zn 0.832 0.148 0.700
Zn 0.633 0.648 0.700
Zn 0.332 0.347 0.700
Zn 0.133 0.847 0.700
Zn 0.832 0.847 0.200
Zn 0.633 0.347 0.200

Zn 0.332 0.648 0.200
Zn 0.133 0.148 0.200
O 0.633 0.347 0.821
O 0.833 0.847 0.821
O 0.333 0.648 0.821
O 0.133 0.148 0.821
O 0.133 0.848 0.321
O 0.332 0.348 0.321
O 0.832 0.148 0.321
O 0.633 0.648 0.321

Str 34 (AEL)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.28 eV
E_{rel}: 0.16 eV/ZnO
$Pore_{max}$: 0.32 nm
V_{pore}: 11 %
D_{pore}: 1
cell parameters
8.832 11.915 5.285 90.01 90.02 89.99
fractional coordinates
Zn 0.526 0.115 0.810
Zn 0.438 0.615 0.810
Zn 0.526 0.393 0.810
Zn 0.438 0.893 0.810
Zn 0.119 0.754 0.810
Zn 0.844 0.254 0.810
Zn 0.835 0.966 0.808
Zn 0.835 0.542 0.808
Zn 0.128 0.466 0.808
Zn 0.128 0.042 0.808
Zn 0.938 0.115 0.310
Zn 0.026 0.615 0.310
Zn 0.026 0.893 0.310
Zn 0.938 0.393 0.310
Zn 0.619 0.254 0.310
Zn 0.344 0.754 0.310
Zn 0.335 0.466 0.308
Zn 0.335 0.042 0.308
Zn 0.628 0.966 0.308
Zn 0.628 0.542 0.308
O 0.341 0.754 0.691
O 0.622 0.254 0.691
O 0.939 0.116 0.687
O 0.939 0.392 0.687
O 0.024 0.892 0.687
O 0.024 0.616 0.687
O 0.628 0.542 0.686
O 0.334 0.466 0.686
O 0.334 0.042 0.686
O 0.628 0.966 0.686
O 0.841 0.254 0.191
O 0.122 0.754 0.191

O 0.439 0.616 0.187
O 0.524 0.392 0.187
O 0.439 0.892 0.187
O 0.524 0.116 0.187
O 0.128 0.042 0.186
O 0.834 0.966 0.186
O 0.835 0.542 0.186
O 0.128 0.466 0.186

Str 35 (APD)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.56 eV
E_{rel}: 0.22 eV/ZnO
$Pore_{max}$: 0.27 nm
V_{pore}: 12 %
D_{pore}: 1
cell parameters
5.281 13.064 6.545 90.00 90.00 90.00
fractional coordinates
Zn 0.312 0.202 0.902
Zn 0.188 0.702 0.902
Zn 0.801 0.052 0.897
Zn 0.699 0.552 0.897
Zn 0.301 0.052 0.603
Zn 0.199 0.552 0.603
Zn 0.812 0.202 0.598
Zn 0.688 0.702 0.598
Zn 0.312 0.298 0.402
Zn 0.188 0.798 0.402
Zn 0.801 0.448 0.397
Zn 0.699 0.948 0.397
Zn 0.301 0.448 0.103
Zn 0.199 0.948 0.103
Zn 0.812 0.298 0.098
Zn 0.688 0.798 0.098
O 0.809 0.701 0.899
O 0.691 0.201 0.899
O 0.301 0.553 0.898
O 0.199 0.053 0.898
O 0.801 0.553 0.602
O 0.699 0.053 0.602
O 0.309 0.701 0.601
O 0.191 0.201 0.601
O 0.809 0.799 0.399
O 0.691 0.299 0.399
O 0.301 0.947 0.398
O 0.199 0.447 0.398
O 0.801 0.947 0.102
O 0.699 0.447 0.102
O 0.309 0.799 0.101
O 0.191 0.299 0.101

Str 36 (LTJ)[17]

$\Delta E_{gap}(PBE_{GW-fit})$: 0.07 eV
E_{rel}: 0.28 eV/ZnO
$Pore_{max}$: 0.24 nm
V_{pore}: 12 %
D_{pore}: 3
cell parameters
5.798 5.817 6.785 90.00 90.00 90.00
fractional coordinates
Zn 0.580 0.089 0.902
Zn 0.080 0.411 0.848
Zn 0.597 0.563 0.648
Zn 0.903 0.063 0.602
Zn 0.420 0.911 0.402
Zn 0.920 0.589 0.348
Zn 0.403 0.437 0.148
Zn 0.097 0.937 0.102
O 0.931 0.099 0.903
O 0.431 0.401 0.847
O 0.589 0.914 0.652
O 0.911 0.414 0.598
O 0.069 0.901 0.403
O 0.569 0.599 0.347
O 0.411 0.086 0.152
O 0.089 0.586 0.098

Str 37 (hUMQ)[20]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.54 eV
E_{rel}: 0.16 eV/ZnO
$Pore_{max}$: 0.26 nm
V_{pore}: 12 %
D_{pore}: 1
cell parameters
9.024 9.021 5.652 90.00 89.97 90.01
fractional coordinates
Zn 0.246 0.905 0.816
Zn 0.100 0.242 0.816
Zn 0.763 0.096 0.816
Zn 0.909 0.759 0.815
Zn 0.600 0.742 0.670
Zn 0.409 0.259 0.670
Zn 0.263 0.596 0.670
Zn 0.746 0.405 0.670
Zn 0.246 0.096 0.316
Zn 0.100 0.759 0.316
Zn 0.763 0.905 0.316
Zn 0.909 0.241 0.316
Zn 0.409 0.742 0.170
Zn 0.600 0.259 0.170
Zn 0.263 0.405 0.170
Zn 0.746 0.596 0.170
O 0.407 0.742 0.814
O 0.602 0.258 0.814

O 0.262 0.403 0.814
O 0.747 0.598 0.814
O 0.102 0.758 0.672
O 0.907 0.242 0.672
O 0.247 0.098 0.672
O 0.762 0.903 0.672
O 0.407 0.258 0.314
O 0.262 0.598 0.314
O 0.602 0.742 0.314
O 0.747 0.403 0.314
O 0.102 0.242 0.172
O 0.247 0.903 0.172
O 0.907 0.758 0.172
O 0.762 0.098 0.172

Str 38 (AFO)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.33 eV
E_{rel}: 0.19 eV/ZnO
$Pore_{max}$: 0.35 nm
V_{pore}: 12 %
D_{pore}: 1
cell parameters
6.268 9.045 5.264 90.00 90.00 110.27
fractional coordinates
Zn 0.559 0.118 0.599
Zn 0.588 0.739 0.598
Zn 0.151 0.739 0.598
Zn 0.177 0.355 0.592
Zn 0.721 0.442 0.591
Zn 0.452 0.905 0.099
Zn 0.860 0.284 0.098
Zn 0.424 0.284 0.098
Zn 0.834 0.668 0.092
Zn 0.291 0.582 0.091
O 0.560 0.121 0.980
O 0.593 0.745 0.976
O 0.178 0.356 0.976
O 0.152 0.745 0.976
O 0.722 0.445 0.970
O 0.451 0.902 0.480
O 0.418 0.278 0.476
O 0.833 0.667 0.476
O 0.860 0.278 0.476
O 0.289 0.578 0.470

Str 39 (ATO)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.23 eV
E_{rel}: 0.18 eV/ZnO
$Pore_{max}$: 0.34 nm
V_{pore}: 12 %
D_{pore}: 1
cell parameters

13.460 13.460 3.213 90.00 90.00 120.00
fractional coordinates
Zn 0.529 0.619 0.925
Zn 0.381 0.910 0.925
Zn 0.090 0.471 0.925
Zn 0.952 0.757 0.742
Zn 0.804 0.048 0.742
Zn 0.243 0.196 0.742
Zn 0.862 0.286 0.591
Zn 0.714 0.577 0.591
Zn 0.423 0.138 0.591
Zn 0.577 0.862 0.408
Zn 0.286 0.423 0.408
Zn 0.138 0.714 0.408
Zn 0.757 0.804 0.258
Zn 0.196 0.952 0.258
Zn 0.048 0.243 0.258
Zn 0.910 0.529 0.075
Zn 0.619 0.090 0.075
Zn 0.471 0.381 0.075
O 0.528 0.911 0.910
O 0.383 0.472 0.910
O 0.089 0.617 0.910
O 0.950 0.194 0.757
O 0.806 0.756 0.757
O 0.244 0.050 0.757
O 0.861 0.578 0.577
O 0.717 0.139 0.577
O 0.422 0.283 0.577
O 0.578 0.717 0.423
O 0.283 0.861 0.423
O 0.139 0.422 0.423
O 0.756 0.950 0.243
O 0.194 0.244 0.243
O 0.050 0.806 0.243
O 0.911 0.383 0.090
O 0.617 0.528 0.090
O 0.472 0.089 0.090

Str 40 (JRY)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.35 eV
E_{rel}: 0.28 eV/ZnO
$Pore_{max}$: 0.25 nm
V_{pore}: 12 %
D_{pore}: 1
cell parameters
5.328 5.868 10.876 90.00 90.00 90.00
fractional coordinates
Zn 0.583 0.595 0.981
Zn 0.133 0.374 0.922
Zn 0.581 0.091 0.824
Zn 0.419 0.591 0.676

Zn 0.867 0.874 0.578
Zn 0.417 0.095 0.519
Zn 0.917 0.405 0.481
Zn 0.367 0.626 0.422
Zn 0.919 0.909 0.324
Zn 0.081 0.409 0.176
Zn 0.633 0.126 0.078
Zn 0.083 0.905 0.019
O 0.439 0.904 0.975
O 0.896 0.127 0.916
O 0.441 0.416 0.826
O 0.559 0.916 0.674
O 0.104 0.627 0.584
O 0.561 0.404 0.525
O 0.061 0.096 0.475
O 0.604 0.873 0.416
O 0.059 0.584 0.326
O 0.941 0.084 0.174
O 0.396 0.373 0.084
O 0.939 0.596 0.025

Str 41 (OSI)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: -0.04 eV
E_{rel}: 0.16 eV/ZnO
$Pore_{max}$: 0.39 nm
V_{pore}: 12 %
D_{pore}: 1
cell parameters
11.732 11.602 3.376 90.00 90.00 90.00
fractional coordinates
Zn 0.715 0.848 0.500
Zn 0.715 0.157 0.500
Zn 0.619 0.502 0.500
Zn 0.381 0.502 0.500
Zn 0.285 0.848 0.500
Zn 0.285 0.157 0.500
Zn 0.000 0.786 0.500
Zn 0.000 0.219 0.500
Zn 0.881 0.002 0.000
Zn 0.785 0.657 0.000
Zn 0.785 0.348 0.000
Zn 0.500 0.719 0.000
Zn 0.500 0.286 0.000
Zn 0.215 0.657 0.000
Zn 0.215 0.348 0.000
Zn 0.119 0.002 0.000
O 0.847 0.714 0.500
O 0.847 0.291 0.500
O 0.788 0.002 0.500
O 0.500 0.626 0.500
O 0.500 0.379 0.500
O 0.212 0.002 0.500

O 0.153 0.714 0.500
O 0.153 0.291 0.500
O 0.712 0.502 0.000
O 0.653 0.791 0.000
O 0.653 0.214 0.000
O 0.347 0.791 0.000
O 0.347 0.214 0.000
O 0.288 0.502 0.000
O 0.000 0.879 0.000
O 0.000 0.126 0.000

Str 42 (MVY)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.26 eV
E_{rel}: 0.39 eV/ZnO
$Pore_{max}$: 0.25 nm
V_{pore}: 13 %
D_{pore}: 1
cell parameters
3.190 5.734 9.195 90.00 90.00 90.00
fractional coordinates
Zn 0.603 0.678 0.796
Zn 0.897 0.178 0.704
Zn 0.233 0.894 0.500
Zn 0.897 0.178 0.296
Zn 0.603 0.678 0.204
Zn 0.267 0.394 0.000
O 0.392 0.317 0.795
O 0.108 0.817 0.705
O 0.718 0.118 0.500
O 0.108 0.817 0.295
O 0.392 0.317 0.205
O 0.782 0.618 0.000

Str 43 AWO)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.50 eV
E_{rel}: 0.25 eV/ZnO
$Pore_{max}$: 0.27 nm
V_{pore}: 13 %
D_{pore}: 3
cell parameters
5.832 10.117 11.881 90.00 90.00 90.20
fractional coordinates
Zn 0.690 0.506 0.919
Zn 0.190 0.006 0.919
Zn 0.674 0.141 0.829
Zn 0.174 0.641 0.829
Zn 0.835 0.844 0.820
Zn 0.335 0.344 0.820
Zn 0.835 0.344 0.680
Zn 0.335 0.844 0.680
Zn 0.674 0.641 0.671
Zn 0.174 0.141 0.671

Zn 0.690 0.006 0.581
Zn 0.190 0.506 0.581
Zn 0.810 0.494 0.419
Zn 0.310 0.994 0.419
Zn 0.826 0.859 0.329
Zn 0.326 0.359 0.329
Zn 0.665 0.156 0.320
Zn 0.165 0.656 0.320
Zn 0.665 0.656 0.180
Zn 0.165 0.156 0.180
Zn 0.826 0.359 0.171
Zn 0.326 0.859 0.171
Zn 0.810 0.994 0.081
Zn 0.310 0.494 0.081
O 0.815 0.002 0.917
O 0.315 0.502 0.917
O 0.688 0.341 0.829
O 0.188 0.841 0.829
O 0.827 0.643 0.828
O 0.327 0.143 0.828
O 0.827 0.143 0.672
O 0.327 0.643 0.672
O 0.688 0.841 0.671
O 0.188 0.341 0.671
O 0.815 0.502 0.583
O 0.315 0.002 0.583
O 0.685 0.998 0.417
O 0.185 0.498 0.417
O 0.812 0.659 0.329
O 0.312 0.159 0.329
O 0.673 0.357 0.328
O 0.173 0.857 0.328
O 0.673 0.857 0.172
O 0.173 0.357 0.172
O 0.812 0.159 0.171
O 0.312 0.659 0.171
O 0.685 0.498 0.083
O 0.185 0.998 0.083

Str 44 (UEI)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.51 eV
E_{rel}: 0.25 eV/ZnO
$Pore_{max}$: 0.30 nm
V_{pore}: 13 %
D_{pore}: 3
cell parameters
11.887 5.859 10.095 90.00 90.00 90.00
fractional coordinates
Zn 0.821 0.333 0.840
Zn 0.679 0.833 0.840
Zn 0.321 0.167 0.840
Zn 0.179 0.667 0.840

Zn 0.828 0.672 0.636
Zn 0.672 0.172 0.636
Zn 0.328 0.828 0.636
Zn 0.172 0.328 0.636
Zn 0.919 0.189 0.501
Zn 0.581 0.689 0.501
Zn 0.419 0.311 0.501
Zn 0.081 0.811 0.501
Zn 0.821 0.833 0.340
Zn 0.679 0.333 0.340
Zn 0.321 0.667 0.340
Zn 0.179 0.167 0.340
Zn 0.828 0.172 0.136
Zn 0.672 0.672 0.136
Zn 0.328 0.328 0.136
Zn 0.172 0.828 0.136
Zn 0.919 0.689 0.001
Zn 0.581 0.189 0.001
Zn 0.419 0.811 0.001
Zn 0.081 0.311 0.001
O 0.917 0.315 0.999
O 0.583 0.815 0.999
O 0.417 0.185 0.999
O 0.083 0.685 0.999
O 0.828 0.684 0.837
O 0.672 0.184 0.837
O 0.328 0.816 0.837
O 0.172 0.316 0.837
O 0.828 0.327 0.639
O 0.672 0.827 0.639
O 0.328 0.173 0.639
O 0.172 0.673 0.639
O 0.917 0.815 0.499
O 0.583 0.315 0.499
O 0.417 0.685 0.499
O 0.083 0.185 0.499
O 0.828 0.184 0.337
O 0.672 0.684 0.337
O 0.328 0.316 0.337
O 0.172 0.816 0.337
O 0.828 0.827 0.139
O 0.672 0.327 0.139
O 0.328 0.673 0.139
O 0.172 0.173 0.139

Str 45 (ATN)[17]
ΔE_{gap}(PBE$_{GW-fit}$): 0.61 eV
E_{rel}: 0.18 eV/ZnO
Pore$_{max}$: 0.34 nm
V_{pore}: 14 %
D_{pore}: 1
cell parameters

8.312 8.312 3.392 90.00 90.00 90.00
fractional coordinates
Zn 0.902 0.731 0.500
Zn 0.727 0.137 0.500
Zn 0.309 0.906 0.500
Zn 0.133 0.313 0.500
Zn 0.809 0.406 0.000
Zn 0.633 0.813 0.000
Zn 0.402 0.231 0.000
Zn 0.227 0.637 0.000
O 0.902 0.310 0.500
O 0.729 0.905 0.500
O 0.306 0.138 0.500
O 0.134 0.733 0.500
O 0.806 0.638 0.000
O 0.634 0.233 0.000
O 0.402 0.810 0.000
O 0.229 0.405 0.000

Str 46 (SAF)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.38 eV
E_{rel}: 0.20 eV/ZnO
$Pore_{max}$: 0.41 nm
V_{pore}: 14 %
D_{pore}: 1
cell parameters
9.513 18.309 5.260 90.00 90.00 90.00
fractional coordinates
Zn 0.902 0.777 0.695
Zn 0.598 0.277 0.695
Zn 0.402 0.723 0.695
Zn 0.098 0.223 0.695
Zn 0.786 0.136 0.692
Zn 0.714 0.636 0.692
Zn 0.286 0.364 0.692
Zn 0.214 0.864 0.692
Zn 0.895 0.948 0.688
Zn 0.605 0.448 0.688
Zn 0.395 0.552 0.688
Zn 0.105 0.052 0.688
Zn 0.899 0.330 0.686
Zn 0.601 0.830 0.686
Zn 0.399 0.170 0.686
Zn 0.101 0.670 0.686
Zn 0.902 0.223 0.195
Zn 0.598 0.723 0.195
Zn 0.402 0.277 0.195
Zn 0.098 0.777 0.195
Zn 0.786 0.864 0.192
Zn 0.714 0.364 0.192
Zn 0.286 0.636 0.192
Zn 0.214 0.136 0.192

Zn 0.895 0.052 0.188
Zn 0.605 0.552 0.188
Zn 0.395 0.448 0.188
Zn 0.105 0.948 0.188
Zn 0.899 0.670 0.186
Zn 0.601 0.170 0.186
Zn 0.399 0.830 0.186
Zn 0.101 0.330 0.186
O 0.897 0.222 0.815
O 0.603 0.722 0.815
O 0.397 0.278 0.815
O 0.103 0.778 0.815
O 0.893 0.051 0.808
O 0.606 0.551 0.808
O 0.394 0.449 0.808
O 0.106 0.949 0.808
O 0.787 0.863 0.808
O 0.713 0.363 0.808
O 0.287 0.637 0.808
O 0.213 0.137 0.808
O 0.902 0.667 0.808
O 0.598 0.167 0.808
O 0.402 0.833 0.808
O 0.098 0.333 0.808
O 0.897 0.778 0.315
O 0.603 0.278 0.315
O 0.397 0.722 0.315
O 0.103 0.222 0.315
O 0.893 0.949 0.308
O 0.606 0.449 0.308
O 0.394 0.551 0.308
O 0.106 0.051 0.308
O 0.787 0.137 0.308
O 0.713 0.637 0.308
O 0.287 0.363 0.308
O 0.213 0.863 0.308
O 0.902 0.333 0.308
O 0.598 0.833 0.308
O 0.402 0.167 0.308
O 0.098 0.667 0.308

Str 47 (APC)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.44 eV
E_{rel}: 0.23 eV/ZnO
$Pore_{max}$: 0.26 nm
V_{pore}: 14 %
D_{pore}: 3
cell parameters
5.788 12.765 6.464 90.00 90.00 90.00
fractional coordinates
Zn 0.328 0.711 0.895
Zn 0.172 0.211 0.895

Zn 0.824 0.048 0.881
Zn 0.676 0.548 0.881
Zn 0.324 0.048 0.619
Zn 0.176 0.548 0.619
Zn 0.828 0.711 0.605
Zn 0.672 0.211 0.605
Zn 0.328 0.789 0.395
Zn 0.172 0.289 0.395
Zn 0.824 0.452 0.381
Zn 0.676 0.952 0.381
Zn 0.324 0.452 0.119
Zn 0.176 0.952 0.119
Zn 0.828 0.789 0.105
Zn 0.672 0.289 0.105
O 0.317 0.549 0.890
O 0.183 0.049 0.890
O 0.822 0.211 0.888
O 0.678 0.711 0.888
O 0.322 0.211 0.612
O 0.178 0.711 0.612
O 0.817 0.549 0.610
O 0.683 0.049 0.610
O 0.317 0.951 0.390
O 0.183 0.451 0.390
O 0.822 0.289 0.388
O 0.678 0.789 0.388
O 0.322 0.289 0.112
O 0.178 0.789 0.112
O 0.817 0.951 0.110
O 0.683 0.451 0.110

Str 48 (CAN)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.48 eV
E_{rel}: 0.15 eV/ZnO
$Pore_{max}$: 0.33 nm
V_{pore}: 14 %
D_{pore}: 1
cell parameters
7.817 7.817 3.368 90.00 90.00 120.00
fractional coordinates
Zn 0.611 0.686 0.750
Zn 0.340 0.933 0.750
Zn 0.094 0.416 0.750
Zn 0.936 0.607 0.250
Zn 0.690 0.090 0.250
Zn 0.419 0.337 0.250
O 0.610 0.932 0.750
O 0.341 0.417 0.750
O 0.094 0.686 0.750
O 0.936 0.337 0.250
O 0.689 0.606 0.250
O 0.420 0.091 0.250

Str 49 (AFG)[17]

$\Delta E_{gap}(PBE_{GW-fit})$: 0.50 eV

E_{rel}: 0.14 eV/ZnO

$Pore_{max}$: 0.33 nm

V_{pore}: 15 %

D_{pore}: 3

cell parameters

7.848 7.849 13.415 90.00 90.00 120.00

fractional coordinates

Zn 0.844 0.426 0.875
Zn 0.573 0.670 0.875
Zn 0.328 0.155 0.875
Zn 0.654 0.076 0.750
Zn 0.168 0.345 0.750
Zn 0.923 0.831 0.750
Zn 0.838 0.417 0.625
Zn 0.582 0.673 0.625
Zn 0.326 0.161 0.625
Zn 0.241 0.489 0.500
Zn 0.995 0.758 0.500
Zn 0.509 0.003 0.500
Zn 0.835 0.408 0.375
Zn 0.590 0.679 0.375
Zn 0.320 0.164 0.375
Zn 0.995 0.758 0.251
Zn 0.509 0.003 0.251
Zn 0.241 0.489 0.250
Zn 0.838 0.417 0.125
Zn 0.582 0.673 0.125
Zn 0.326 0.161 0.125
Zn 0.923 0.831 0.000
Zn 0.654 0.076 0.000
Zn 0.168 0.345 0.000
O 0.842 0.670 0.875
O 0.575 0.157 0.875
O 0.328 0.424 0.875
O 0.923 0.345 0.751
O 0.654 0.831 0.751
O 0.168 0.075 0.751
O 0.836 0.672 0.625
O 0.582 0.162 0.625
O 0.327 0.417 0.625
O 0.510 0.759 0.500
O 0.240 0.003 0.500
O 0.995 0.489 0.500
O 0.835 0.677 0.375
O 0.589 0.164 0.375
O 0.321 0.410 0.375
O 0.995 0.489 0.251
O 0.240 0.003 0.251
O 0.510 0.759 0.251

O 0.836 0.672 0.125
O 0.582 0.162 0.125
O 0.327 0.417 0.125
O 0.168 0.075 0.000
O 0.654 0.831 0.000
O 0.923 0.345 0.000

Str 50 (TOL)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.49 eV
E_{rel}: 0.14 eV/ZnO
$Pore_{max}$: 0.33 nm
V_{pore}: 15 %
D_{pore}: 3
cell parameters
7.863 7.863 20.073 90.00 90.00 120.00
fractional coordinates
Zn 0.748 0.746 1.000
Zn 0.258 0.002 1.000
Zn 0.003 0.257 1.000
Zn 0.588 0.928 0.917
Zn 0.344 0.416 0.917
Zn 0.077 0.661 0.917
Zn 0.748 0.747 0.833
Zn 0.258 0.002 0.833
Zn 0.003 0.257 0.833
Zn 0.930 0.587 0.750
Zn 0.662 0.075 0.750
Zn 0.418 0.343 0.750
Zn 0.748 0.747 0.666
Zn 0.258 0.002 0.666
Zn 0.003 0.257 0.666
Zn 0.344 0.416 0.583
Zn 0.589 0.929 0.583
Zn 0.076 0.661 0.583
Zn 0.750 0.740 0.500
Zn 0.995 0.255 0.500
Zn 0.265 0.010 0.500
Zn 0.589 0.929 0.417
Zn 0.344 0.416 0.417
Zn 0.076 0.661 0.417
Zn 0.748 0.746 0.333
Zn 0.259 0.002 0.333
Zn 0.003 0.257 0.333
Zn 0.930 0.588 0.250
Zn 0.662 0.075 0.250
Zn 0.417 0.343 0.250
Zn 0.742 0.749 0.167
Zn 0.256 0.993 0.167
Zn 0.011 0.263 0.167
Zn 0.662 0.074 0.083
Zn 0.930 0.588 0.083
Zn 0.417 0.343 0.083

O 0.257 0.256 1.000
O 0.749 0.002 1.000
O 0.003 0.748 1.000
O 0.589 0.660 0.917
O 0.345 0.930 0.917
O 0.075 0.416 0.917
O 0.257 0.256 0.833
O 0.749 0.002 0.833
O 0.003 0.747 0.833
O 0.661 0.587 0.750
O 0.417 0.074 0.750
O 0.931 0.344 0.750
O 0.257 0.256 0.666
O 0.749 0.002 0.666
O 0.003 0.747 0.666
O 0.589 0.660 0.583
O 0.345 0.929 0.583
O 0.076 0.416 0.583
O 0.750 0.009 0.500
O 0.263 0.254 0.500
O 0.996 0.742 0.500
O 0.589 0.660 0.417
O 0.345 0.929 0.417
O 0.076 0.416 0.417
O 0.257 0.256 0.333
O 0.003 0.748 0.333
O 0.749 0.002 0.333
O 0.662 0.587 0.250
O 0.930 0.343 0.250
O 0.417 0.074 0.250
O 0.743 0.995 0.167
O 0.010 0.749 0.167
O 0.256 0.262 0.167
O 0.930 0.343 0.083
O 0.417 0.074 0.083
O 0.662 0.587 0.083

Str 51 (LIO)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.50 eV
E_{rel}: 0.14 eV/ZnO
$Pore_{max}$: 0.33 nm
V_{pore}: 15 %
D_{pore}: 3
cell parameters
7.857 7.857 10.050 90.00 90.00 120.01
fractional coordinates
Zn 0.080 0.411 0.833
Zn 0.336 0.921 0.833
Zn 0.590 0.666 0.833
Zn 0.921 0.593 0.667
Zn 0.677 0.080 0.667
Zn 0.408 0.324 0.667

Zn 0.597 0.674 0.500
Zn 0.327 0.919 0.500
Zn 0.082 0.404 0.500
Zn 0.677 0.080 0.334
Zn 0.408 0.324 0.334
Zn 0.921 0.593 0.334
Zn 0.590 0.666 0.167
Zn 0.336 0.921 0.167
Zn 0.080 0.411 0.167
Zn 0.994 0.740 0.000
Zn 0.750 0.007 0.000
Zn 0.262 0.251 0.000
O 0.081 0.666 0.834
O 0.590 0.920 0.833
O 0.335 0.411 0.833
O 0.922 0.325 0.666
O 0.677 0.593 0.666
O 0.408 0.080 0.666
O 0.596 0.919 0.500
O 0.082 0.673 0.500
O 0.328 0.405 0.500
O 0.677 0.593 0.334
O 0.408 0.080 0.334
O 0.922 0.325 0.334
O 0.335 0.411 0.167
O 0.590 0.920 0.167
O 0.081 0.666 0.167
O 0.994 0.252 0.000
O 0.264 0.008 0.000
O 0.749 0.738 0.000

Str 52 (LOS)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.49 eV
E_{rel}: 0.14 eV/ZnO
$Pore_{max}$: 0.34 nm
V_{pore}: 15 %
D_{pore}: 3
cell parameters
7.887 7.887 6.670 90.00 90.00 120.00
fractional coordinates
Zn 0.587 0.935 0.750
Zn 0.344 0.424 0.750
Zn 0.076 0.667 0.750
Zn 0.748 0.755 0.500
Zn 0.256 0.009 0.500
Zn 0.002 0.263 0.500
Zn 0.928 0.594 0.250
Zn 0.660 0.083 0.250
Zn 0.417 0.350 0.250
Zn 0.748 0.755 0.000
Zn 0.256 0.009 0.000
Zn 0.002 0.263 0.000

O 0.587 0.667 0.750
O 0.344 0.936 0.750
O 0.075 0.424 0.750
O 0.748 0.009 0.500
O 0.256 0.263 0.500
O 0.002 0.755 0.500
O 0.929 0.351 0.250
O 0.660 0.594 0.250
O 0.417 0.082 0.250
O 0.748 0.009 0.000
O 0.256 0.263 0.000
O 0.002 0.755 0.000

Str 53 (SOD)[17]
ΔE_{gap}(PBE$_{GW-fit}$): 0.53 eV
E_{rel}: 0.14 eV/ZnO
Pore$_{max}$: 0.35 nm
V_{pore}: 15 %
D_{pore}: 3
cell parameters
5.663 5.663 5.663 90.00 90.00 90.00
fractional coordinates
Zn 0.000 0.500 0.750
Zn 0.750 0.000 0.500
Zn 0.250 0.000 0.500
Zn 0.000 0.500 0.250
Zn 0.500 0.750 0.000
Zn 0.500 0.250 0.000
O 0.500 0.000 0.750
O 0.000 0.750 0.500
O 0.000 0.250 0.500
O 0.500 0.000 0.250
O 0.750 0.500 0.000
O 0.250 0.500 0.000

Str 54 (AET)[17]
ΔE_{gap}(PBE$_{GW-fit}$): 0.45 eV
E_{rel}: 0.23 eV/ZnO
Pore$_{max}$: 0.41 nm
V_{pore}: 17 %
D_{pore}: 1
cell parameters
21.516 9.431 5.296 90.00 90.00 90.00
fractional coordinates
Zn 0.500 0.352 0.583
Zn 0.000 0.852 0.583
Zn 0.819 0.399 0.563
Zn 0.681 0.899 0.563
Zn 0.319 0.899 0.563
Zn 0.181 0.399 0.563
Zn 0.921 0.111 0.563
Zn 0.579 0.611 0.563

Zn 0.421 0.611 0.563
Zn 0.079 0.111 0.563
Zn 0.846 0.790 0.560
Zn 0.654 0.290 0.560
Zn 0.346 0.290 0.560
Zn 0.154 0.790 0.560
Zn 0.772 0.099 0.554
Zn 0.728 0.599 0.554
Zn 0.272 0.599 0.554
Zn 0.228 0.099 0.554
Zn 0.500 0.648 0.083
Zn 0.000 0.148 0.083
Zn 0.819 0.601 0.063
Zn 0.681 0.101 0.063
Zn 0.319 0.101 0.063
Zn 0.181 0.601 0.063
Zn 0.921 0.889 0.063
Zn 0.579 0.389 0.063
Zn 0.421 0.389 0.063
Zn 0.079 0.889 0.063
Zn 0.846 0.210 0.060
Zn 0.654 0.710 0.060
Zn 0.346 0.710 0.060
Zn 0.154 0.210 0.060
Zn 0.772 0.901 0.054
Zn 0.728 0.401 0.054
Zn 0.272 0.401 0.054
Zn 0.228 0.901 0.054
O 0.920 0.102 0.940
O 0.580 0.602 0.940
O 0.420 0.602 0.940
O 0.080 0.102 0.940
O 0.845 0.790 0.939
O 0.655 0.290 0.939
O 0.345 0.290 0.939
O 0.155 0.790 0.939
O 0.822 0.401 0.939
O 0.678 0.901 0.939
O 0.322 0.901 0.939
O 0.178 0.401 0.939
O 0.500 0.320 0.937
O 0.000 0.820 0.937
O 0.772 0.103 0.931
O 0.728 0.603 0.931
O 0.272 0.603 0.931
O 0.228 0.103 0.931
O 0.920 0.898 0.440
O 0.580 0.398 0.440
O 0.420 0.398 0.440
O 0.080 0.898 0.440
O 0.845 0.210 0.439
O 0.655 0.710 0.439

O 0.345 0.710 0.439
O 0.155 0.210 0.439
O 0.822 0.599 0.439
O 0.678 0.099 0.439
O 0.322 0.099 0.439
O 0.178 0.599 0.439
O 0.500 0.680 0.437
O 0.000 0.180 0.437
O 0.772 0.897 0.431
O 0.728 0.397 0.431
O 0.272 0.397 0.431
O 0.228 0.897 0.431

Str 55 (ATT)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.65 eV
E_{rel}: 0.29 eV/ZnO
$Pore_{max}$: 0.28 nm
V_{pore}: 17 %
D_{pore}: 2
cell parameters
6.223 10.376 5.707 90.00 90.00 90.00
fractional coordinates
Zn 0.926 0.750 0.858
Zn 0.574 0.250 0.858
Zn 0.910 0.401 0.641
Zn 0.910 0.099 0.641
Zn 0.590 0.901 0.641
Zn 0.590 0.599 0.641
Zn 0.410 0.401 0.359
Zn 0.410 0.099 0.359
Zn 0.090 0.901 0.359
Zn 0.090 0.599 0.359
Zn 0.426 0.750 0.142
Zn 0.074 0.250 0.142
O 0.920 0.250 0.851
O 0.580 0.750 0.851
O 0.923 0.904 0.653
O 0.923 0.596 0.653
O 0.577 0.404 0.653
O 0.577 0.096 0.653
O 0.423 0.904 0.347
O 0.423 0.596 0.347
O 0.077 0.404 0.347
O 0.077 0.096 0.347
O 0.420 0.250 0.149
O 0.080 0.750 0.149

Str 56 (ACO)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.99 eV
E_{rel}: 0.23 eV/ZnO
$Pore_{max}$: 0.23 nm
V_{pore}: 17 %

D_{pore}: 3
cell parameters
6.278 6.278 6.278 90.00 90.00 90.00
fractional coordinates
Zn 0.835 0.165 0.835
Zn 0.165 0.835 0.835
Zn 0.665 0.665 0.665
Zn 0.335 0.335 0.665
Zn 0.665 0.335 0.335
Zn 0.335 0.665 0.335
Zn 0.835 0.835 0.165
Zn 0.165 0.165 0.165
O 0.838 0.838 0.838
O 0.162 0.162 0.838
O 0.662 0.338 0.662
O 0.338 0.662 0.662
O 0.662 0.662 0.338
O 0.338 0.338 0.338
O 0.838 0.162 0.162
O 0.162 0.838 0.162

Str 57 (PON)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.33 eV
E_{rel}: 0.31 eV/ZnO
$Pore_{max}$: 0.30 nm
V_{pore}: 17 %
D_{pore}: 2
cell parameters
5.881 5.945 10.455 90.00 90.00 90.00
fractional coordinates
Zn 0.838 0.142 0.894
Zn 0.338 0.858 0.894
Zn 0.812 0.605 0.836
Zn 0.312 0.395 0.836
Zn 0.971 0.358 0.578
Zn 0.471 0.642 0.578
Zn 0.662 0.142 0.394
Zn 0.162 0.858 0.394
Zn 0.688 0.605 0.336
Zn 0.188 0.395 0.336
Zn 0.529 0.358 0.078
Zn 0.029 0.642 0.078
O 0.990 0.858 0.910
O 0.490 0.142 0.910
O 0.507 0.654 0.761
O 0.007 0.346 0.761
O 0.675 0.417 0.503
O 0.175 0.583 0.503
O 0.510 0.858 0.410
O 0.010 0.142 0.410
O 0.993 0.654 0.261
O 0.493 0.346 0.261

O 0.825 0.417 0.003
O 0.325 0.583 0.003

Str 58 (ZON)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.59 eV
E_{rel}: 0.31 eV/ZnO
$Pore_{max}$: 0.32 nm
V_{pore}: 18 %
D_{pore}: 2
cell parameters
9.108 9.988 10.863 90.00 90.00 90.00
fractional coordinates
Zn 0.769 0.341 0.965
Zn 0.731 0.841 0.965
Zn 0.927 0.098 0.929
Zn 0.573 0.598 0.929
Zn 0.425 0.901 0.924
Zn 0.075 0.401 0.924
Zn 0.433 0.273 0.834
Zn 0.067 0.773 0.834
Zn 0.933 0.273 0.666
Zn 0.567 0.773 0.666
Zn 0.925 0.901 0.576
Zn 0.575 0.401 0.576
Zn 0.427 0.098 0.571
Zn 0.073 0.598 0.571
Zn 0.270 0.341 0.535
Zn 0.231 0.841 0.535
Zn 0.769 0.159 0.465
Zn 0.731 0.659 0.465
Zn 0.927 0.402 0.429
Zn 0.573 0.902 0.429
Zn 0.425 0.599 0.424
Zn 0.075 0.099 0.424
Zn 0.433 0.227 0.334
Zn 0.067 0.727 0.334
Zn 0.933 0.227 0.166
Zn 0.567 0.727 0.166
Zn 0.925 0.599 0.076
Zn 0.575 0.099 0.076
Zn 0.427 0.402 0.071
Zn 0.073 0.902 0.071
Zn 0.270 0.159 0.035
Zn 0.231 0.659 0.035
O 0.272 0.339 0.949
O 0.228 0.839 0.949
O 0.434 0.098 0.924
O 0.066 0.598 0.924
O 0.921 0.904 0.918
O 0.579 0.404 0.918
O 0.935 0.271 0.842
O 0.565 0.771 0.842

O 0.435 0.271 0.658
O 0.065 0.771 0.658
O 0.421 0.904 0.582
O 0.079 0.404 0.582
O 0.934 0.098 0.576
O 0.566 0.598 0.576
O 0.772 0.339 0.551
O 0.728 0.839 0.551
O 0.272 0.161 0.449
O 0.228 0.661 0.449
O 0.434 0.402 0.424
O 0.066 0.902 0.424
O 0.921 0.596 0.418
O 0.579 0.096 0.418
O 0.935 0.229 0.342
O 0.565 0.729 0.342
O 0.435 0.229 0.158
O 0.065 0.729 0.158
O 0.421 0.596 0.082
O 0.079 0.096 0.082
O 0.934 0.402 0.076
O 0.566 0.902 0.076
O 0.772 0.161 0.051
O 0.728 0.661 0.051

Str 59 (OWE)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.68 eV
E_{rel}: 0.36 eV/ZnO
$Pore_{max}$: 0.30 nm
V_{pore}: 18 %
D_{pore}: 2
cell parameters
9.477 9.404 5.534 90.00 90.00 90.00
fractional coordinates
Zn 0.981 0.250 0.833
Zn 0.519 0.750 0.833
Zn 0.861 0.899 0.645
Zn 0.861 0.601 0.645
Zn 0.639 0.399 0.645
Zn 0.639 0.101 0.645
Zn 0.355 0.250 0.620
Zn 0.145 0.750 0.620
Zn 0.855 0.250 0.380
Zn 0.645 0.750 0.380
Zn 0.361 0.899 0.355
Zn 0.361 0.601 0.355
Zn 0.139 0.399 0.355
Zn 0.139 0.101 0.355
Zn 0.481 0.250 0.167
Zn 0.019 0.750 0.167
O 0.979 0.750 0.824
O 0.521 0.250 0.824

O 0.863 0.398 0.661
O 0.863 0.102 0.661
O 0.637 0.898 0.661
O 0.637 0.602 0.661
O 0.349 0.750 0.625
O 0.151 0.250 0.625
O 0.849 0.750 0.375
O 0.651 0.250 0.375
O 0.363 0.398 0.339
O 0.363 0.102 0.339
O 0.137 0.898 0.339
O 0.137 0.602 0.339
O 0.479 0.750 0.176
O 0.021 0.250 0.176

Str 60 (AFI)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.48 eV
E_{rel}: 0.19 eV/ZnO
$Pore_{max}$: 0.48 nm
V_{pore}: 18 %
D_{pore}: 1
cell parameters
8.925 8.925 5.298 90.00 90.00 120.00
fractional coordinates
Zn 0.877 0.326 0.688
Zn 0.674 0.551 0.688
Zn 0.551 0.877 0.688
Zn 0.449 0.123 0.688
Zn 0.326 0.449 0.688
Zn 0.123 0.674 0.688
Zn 0.877 0.551 0.188
Zn 0.674 0.123 0.188
Zn 0.551 0.674 0.188
Zn 0.449 0.326 0.188
Zn 0.326 0.877 0.188
Zn 0.123 0.449 0.188
O 0.878 0.552 0.812
O 0.674 0.122 0.812
O 0.552 0.674 0.812
O 0.448 0.326 0.812
O 0.326 0.878 0.812
O 0.122 0.448 0.812
O 0.878 0.326 0.312
O 0.674 0.552 0.312
O 0.552 0.878 0.312
O 0.448 0.122 0.312
O 0.326 0.448 0.312
O 0.122 0.674 0.312

Str 61 (LAU)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.29 eV
E_{rel}: 0.32 eV/ZnO

$Pore_{max}$: 0.33 nm
V_{pore}: 19 %
D_{pore}: 2
cell parameters
9.018 8.426 10.503 90.00 112.56 90.00
fractional coordinates
Zn 0.614 0.377 0.944
Zn 0.114 0.877 0.944
Zn 0.881 0.185 0.869
Zn 0.381 0.685 0.869
Zn 0.742 0.618 0.826
Zn 0.242 0.118 0.826
Zn 0.758 0.882 0.674
Zn 0.258 0.382 0.674
Zn 0.619 0.315 0.631
Zn 0.119 0.815 0.631
Zn 0.886 0.123 0.556
Zn 0.386 0.623 0.556
Zn 0.614 0.623 0.444
Zn 0.114 0.123 0.444
Zn 0.881 0.815 0.369
Zn 0.381 0.315 0.369
Zn 0.742 0.382 0.326
Zn 0.242 0.882 0.326
Zn 0.758 0.118 0.174
Zn 0.258 0.618 0.174
Zn 0.619 0.685 0.131
Zn 0.119 0.185 0.131
Zn 0.886 0.877 0.056
Zn 0.386 0.377 0.056
O 0.612 0.622 0.943
O 0.112 0.122 0.943
O 0.879 0.809 0.870
O 0.379 0.309 0.870
O 0.742 0.381 0.828
O 0.242 0.881 0.828
O 0.758 0.119 0.672
O 0.258 0.619 0.672
O 0.621 0.691 0.630
O 0.121 0.191 0.630
O 0.888 0.878 0.557
O 0.388 0.378 0.557
O 0.612 0.378 0.443
O 0.112 0.878 0.443
O 0.879 0.191 0.370
O 0.379 0.691 0.370
O 0.742 0.619 0.328
O 0.242 0.119 0.328
O 0.758 0.881 0.172
O 0.258 0.381 0.172
O 0.621 0.309 0.130
O 0.121 0.809 0.130

O 0.888 0.122 0.057
O 0.388 0.622 0.057

Str 62 (GIS)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.52 eV
E_{rel}: 0.29 eV/ZnO
$Pore_{max}$: 0.29 nm
V_{pore}: 21 %
D_{pore}: 3
cell parameters
6.409 6.409 6.327 90.00 90.00 88.87
fractional coordinates
Zn 0.837 0.413 0.875
Zn 0.163 0.087 0.875
Zn 0.663 0.087 0.625
Zn 0.337 0.413 0.625
Zn 0.663 0.587 0.375
Zn 0.337 0.913 0.375
Zn 0.837 0.913 0.125
Zn 0.163 0.587 0.125
O 0.838 0.088 0.875
O 0.162 0.412 0.875
O 0.662 0.412 0.625
O 0.338 0.088 0.625
O 0.662 0.912 0.375
O 0.338 0.588 0.375
O 0.838 0.588 0.125
O 0.162 0.912 0.125

Str 63 (SIV)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.65 eV
E_{rel}: 0.29 eV/ZnO
$Pore_{max}$: 0.32 nm
V_{pore}: 21 %
D_{pore}: 3
cell parameters
6.403 9.010 18.048 90.00 90.65 90.00
fractional coordinates
Zn 0.663 0.520 0.947
Zn 0.163 0.020 0.947
Zn 0.664 0.144 0.884
Zn 0.164 0.644 0.884
Zn 0.838 0.856 0.866
Zn 0.338 0.356 0.866
Zn 0.840 0.478 0.804
Zn 0.340 0.978 0.804
Zn 0.660 0.978 0.696
Zn 0.160 0.478 0.696
Zn 0.662 0.356 0.634
Zn 0.162 0.856 0.634
Zn 0.836 0.644 0.616
Zn 0.336 0.144 0.616

Zn 0.837 0.020 0.553
Zn 0.337 0.520 0.553
Zn 0.663 0.480 0.447
Zn 0.163 0.980 0.447
Zn 0.664 0.856 0.384
Zn 0.164 0.356 0.384
Zn 0.838 0.144 0.366
Zn 0.338 0.644 0.366
Zn 0.840 0.522 0.304
Zn 0.340 0.022 0.304
Zn 0.660 0.022 0.196
Zn 0.160 0.522 0.196
Zn 0.662 0.644 0.134
Zn 0.162 0.144 0.134
Zn 0.836 0.356 0.116
Zn 0.336 0.856 0.116
Zn 0.837 0.980 0.053
Zn 0.337 0.480 0.053
O 0.837 0.019 0.947
O 0.337 0.519 0.947
O 0.837 0.643 0.884
O 0.337 0.143 0.884
O 0.662 0.356 0.867
O 0.162 0.856 0.867
O 0.664 0.981 0.803
O 0.164 0.481 0.803
O 0.836 0.481 0.697
O 0.336 0.981 0.697
O 0.838 0.856 0.633
O 0.338 0.356 0.633
O 0.663 0.143 0.616
O 0.163 0.643 0.616
O 0.663 0.519 0.553
O 0.163 0.019 0.553
O 0.837 0.981 0.447
O 0.337 0.481 0.447
O 0.837 0.357 0.384
O 0.337 0.857 0.384
O 0.662 0.644 0.367
O 0.162 0.144 0.367
O 0.664 0.019 0.303
O 0.164 0.519 0.303
O 0.836 0.519 0.197
O 0.336 0.019 0.197
O 0.838 0.144 0.133
O 0.338 0.644 0.133
O 0.663 0.857 0.116
O 0.163 0.357 0.116
O 0.663 0.481 0.053
O 0.163 0.981 0.053

Str 64 (OFF)[17]

ΔE_{gap}(PBE$_{GW-fit}$): 0.88 eV
E_{rel}: 0.29 eV/ZnO
Pore$_{max}$: 0.37 nm
V_{pore}: 21 %
D_{pore}: 3
cell parameters
8.036 8.036 10.395 90.00 90.00 120.00
fractional coordinates
Zn 0.998 0.249 0.902
Zn 0.751 0.749 0.902
Zn 0.251 0.002 0.902
Zn 0.582 0.931 0.750
Zn 0.348 0.418 0.750
Zn 0.069 0.652 0.750
Zn 0.998 0.249 0.598
Zn 0.751 0.749 0.598
Zn 0.251 0.002 0.598
Zn 0.998 0.749 0.402
Zn 0.751 0.002 0.402
Zn 0.251 0.249 0.402
Zn 0.582 0.652 0.250
Zn 0.348 0.931 0.250
Zn 0.069 0.418 0.250
Zn 0.998 0.749 0.098
Zn 0.751 0.002 0.098
Zn 0.251 0.249 0.098
O 0.993 0.741 0.904
O 0.748 0.007 0.904
O 0.259 0.252 0.904
O 0.582 0.660 0.750
O 0.340 0.922 0.750
O 0.078 0.418 0.750
O 0.993 0.741 0.596
O 0.748 0.007 0.596
O 0.259 0.252 0.596
O 0.993 0.252 0.404
O 0.748 0.741 0.404
O 0.259 0.007 0.404
O 0.582 0.922 0.250
O 0.340 0.418 0.250
O 0.078 0.660 0.250
O 0.993 0.252 0.096
O 0.748 0.741 0.096
O 0.259 0.007 0.096

Str 65 (MOZ)[17]
ΔE_{gap}(PBE$_{GW-fit}$): 0.72 eV
E_{rel}: 0.32 eV/ZnO
Pore$_{max}$: 0.65 nm
V_{pore}: 21 %
D_{pore}: 3
cell parameters

19.478 19.478 10.531 90.00 90.00 120.00
fractional coordinates
Zn 0.908 0.711 0.903
Zn 0.803 0.092 0.903
Zn 0.711 0.803 0.903
Zn 0.289 0.197 0.903
Zn 0.197 0.908 0.903
Zn 0.092 0.289 0.903
Zn 0.802 0.503 0.903
Zn 0.701 0.198 0.903
Zn 0.503 0.701 0.903
Zn 0.497 0.299 0.903
Zn 0.299 0.802 0.903
Zn 0.198 0.497 0.903
Zn 0.906 0.298 0.902
Zn 0.702 0.608 0.902
Zn 0.608 0.906 0.902
Zn 0.392 0.094 0.902
Zn 0.298 0.392 0.902
Zn 0.094 0.702 0.902
Zn 0.945 0.165 0.750
Zn 0.944 0.579 0.750
Zn 0.835 0.779 0.750
Zn 0.834 0.369 0.750
Zn 0.779 0.945 0.750
Zn 0.635 0.056 0.750
Zn 0.631 0.465 0.750
Zn 0.579 0.635 0.750
Zn 0.535 0.166 0.750
Zn 0.465 0.834 0.750
Zn 0.421 0.365 0.750
Zn 0.369 0.535 0.750
Zn 0.365 0.944 0.750
Zn 0.221 0.055 0.750
Zn 0.166 0.631 0.750
Zn 0.165 0.221 0.750
Zn 0.056 0.421 0.750
Zn 0.055 0.835 0.750
Zn 0.906 0.298 0.598
Zn 0.702 0.608 0.598
Zn 0.608 0.906 0.598
Zn 0.392 0.094 0.598
Zn 0.298 0.392 0.598
Zn 0.094 0.702 0.598
Zn 0.802 0.503 0.597
Zn 0.701 0.198 0.597
Zn 0.503 0.701 0.597
Zn 0.497 0.299 0.597
Zn 0.299 0.802 0.597
Zn 0.198 0.497 0.597
Zn 0.908 0.711 0.597
Zn 0.803 0.092 0.597

Zn 0.711 0.803 0.597
Zn 0.289 0.197 0.597
Zn 0.197 0.908 0.597
Zn 0.092 0.289 0.597
Zn 0.908 0.197 0.403
Zn 0.803 0.711 0.403
Zn 0.711 0.908 0.403
Zn 0.289 0.092 0.403
Zn 0.197 0.289 0.403
Zn 0.092 0.803 0.403
Zn 0.802 0.299 0.403
Zn 0.701 0.503 0.403
Zn 0.503 0.802 0.403
Zn 0.497 0.198 0.403
Zn 0.299 0.497 0.403
Zn 0.198 0.701 0.403
Zn 0.906 0.608 0.402
Zn 0.702 0.094 0.402
Zn 0.608 0.702 0.402
Zn 0.392 0.298 0.402
Zn 0.298 0.906 0.402
Zn 0.094 0.392 0.402
Zn 0.945 0.779 0.250
Zn 0.944 0.365 0.250
Zn 0.835 0.055 0.250
Zn 0.834 0.465 0.250
Zn 0.779 0.835 0.250
Zn 0.635 0.579 0.250
Zn 0.631 0.166 0.250
Zn 0.579 0.944 0.250
Zn 0.535 0.369 0.250
Zn 0.465 0.631 0.250
Zn 0.421 0.056 0.250
Zn 0.369 0.834 0.250
Zn 0.365 0.421 0.250
Zn 0.221 0.165 0.250
Zn 0.166 0.535 0.250
Zn 0.165 0.945 0.250
Zn 0.056 0.635 0.250
Zn 0.055 0.221 0.250
Zn 0.906 0.608 0.098
Zn 0.702 0.094 0.098
Zn 0.608 0.702 0.098
Zn 0.392 0.298 0.098
Zn 0.298 0.906 0.098
Zn 0.094 0.392 0.098
Zn 0.802 0.299 0.097
Zn 0.701 0.503 0.097
Zn 0.503 0.802 0.097
Zn 0.497 0.198 0.097
Zn 0.299 0.497 0.097
Zn 0.198 0.701 0.097

Zn 0.908 0.197 0.097
Zn 0.803 0.711 0.097
Zn 0.711 0.908 0.097
Zn 0.289 0.092 0.097
Zn 0.197 0.289 0.097
Zn 0.092 0.803 0.097
O 0.908 0.610 0.906
O 0.702 0.092 0.906
O 0.610 0.702 0.906
O 0.390 0.298 0.906
O 0.298 0.908 0.906
O 0.092 0.390 0.906
O 0.911 0.199 0.905
O 0.801 0.712 0.905
O 0.712 0.911 0.905
O 0.288 0.089 0.905
O 0.199 0.288 0.905
O 0.089 0.801 0.905
O 0.800 0.302 0.904
O 0.698 0.499 0.904
O 0.501 0.200 0.904
O 0.499 0.800 0.904
O 0.302 0.501 0.904
O 0.200 0.698 0.904
O 0.942 0.367 0.750
O 0.941 0.781 0.750
O 0.841 0.059 0.750
O 0.838 0.470 0.750
O 0.781 0.841 0.750
O 0.633 0.574 0.750
O 0.632 0.162 0.750
O 0.574 0.942 0.750
O 0.530 0.368 0.750
O 0.470 0.632 0.750
O 0.426 0.058 0.750
O 0.368 0.838 0.750
O 0.367 0.426 0.750
O 0.219 0.159 0.750
O 0.162 0.530 0.750
O 0.159 0.941 0.750
O 0.059 0.219 0.750
O 0.058 0.633 0.750
O 0.800 0.302 0.596
O 0.698 0.499 0.596
O 0.501 0.200 0.596
O 0.499 0.800 0.596
O 0.302 0.501 0.596
O 0.200 0.698 0.596
O 0.911 0.199 0.595
O 0.801 0.712 0.595
O 0.712 0.911 0.595
O 0.288 0.089 0.595

O 0.199 0.288 0.595
O 0.089 0.801 0.595
O 0.908 0.610 0.594
O 0.702 0.092 0.594
O 0.610 0.702 0.594
O 0.390 0.298 0.594
O 0.298 0.908 0.594
O 0.092 0.390 0.594
O 0.908 0.298 0.406
O 0.702 0.610 0.406
O 0.610 0.908 0.406
O 0.390 0.092 0.406
O 0.298 0.390 0.406
O 0.092 0.702 0.406
O 0.911 0.712 0.405
O 0.801 0.089 0.405
O 0.712 0.801 0.405
O 0.288 0.199 0.405
O 0.199 0.911 0.405
O 0.089 0.288 0.405
O 0.800 0.499 0.404
O 0.698 0.200 0.404
O 0.501 0.302 0.404
O 0.499 0.698 0.404
O 0.302 0.800 0.404
O 0.200 0.501 0.404
O 0.942 0.574 0.250
O 0.941 0.159 0.250
O 0.841 0.781 0.250
O 0.838 0.368 0.250
O 0.781 0.941 0.250
O 0.633 0.058 0.250
O 0.632 0.470 0.250
O 0.574 0.633 0.250
O 0.530 0.162 0.250
O 0.470 0.838 0.250
O 0.426 0.367 0.250
O 0.368 0.530 0.250
O 0.367 0.942 0.250
O 0.219 0.059 0.250
O 0.162 0.632 0.250
O 0.159 0.219 0.250
O 0.059 0.841 0.250
O 0.058 0.426 0.250
O 0.800 0.499 0.096
O 0.698 0.200 0.096
O 0.501 0.302 0.096
O 0.499 0.698 0.096
O 0.302 0.800 0.096
O 0.200 0.501 0.096
O 0.911 0.712 0.095
O 0.801 0.089 0.095

O 0.712 0.801 0.095
O 0.288 0.199 0.095
O 0.199 0.911 0.095
O 0.089 0.288 0.095
O 0.908 0.298 0.094
O 0.702 0.610 0.094
O 0.610 0.908 0.094
O 0.390 0.092 0.094
O 0.298 0.390 0.094
O 0.092 0.702 0.094

Str 66 (PHI)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.81 eV
E_{rel}: 0.29 eV/ZnO
$Pore_{max}$: 0.32 nm
V_{pore}: 21 %
D_{pore}: 3
cell parameters
6.418 9.026 9.030 90.00 90.59 90.00
fractional coordinates
Zn 0.837 0.106 0.983
Zn 0.337 0.606 0.983
Zn 0.340 0.227 0.858
Zn 0.840 0.727 0.858
Zn 0.660 0.227 0.642
Zn 0.160 0.727 0.642
Zn 0.663 0.606 0.517
Zn 0.163 0.106 0.517
Zn 0.837 0.894 0.483
Zn 0.337 0.394 0.483
Zn 0.840 0.273 0.358
Zn 0.340 0.773 0.358
Zn 0.660 0.773 0.142
Zn 0.160 0.273 0.142
Zn 0.663 0.394 0.017
Zn 0.163 0.894 0.017
O 0.663 0.607 0.986
O 0.163 0.107 0.986
O 0.664 0.230 0.857
O 0.165 0.730 0.857
O 0.835 0.730 0.643
O 0.336 0.230 0.643
O 0.837 0.107 0.514
O 0.337 0.607 0.514
O 0.663 0.393 0.486
O 0.163 0.893 0.486
O 0.664 0.770 0.357
O 0.165 0.270 0.357
O 0.835 0.270 0.143
O 0.336 0.770 0.143
O 0.837 0.893 0.014
O 0.337 0.393 0.014

Str 67 (MER)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.86 eV
E_{rel}: 0.30 eV/ZnO
$Pore_{max}$: 0.39 nm
V_{pore}: 21 %
D_{pore}: 3
cell parameters
9.046 9.046 6.425 90.00 90.00 90.00
fractional coordinates
Zn 0.893 0.731 0.839
Zn 0.731 0.107 0.839
Zn 0.269 0.893 0.839
Zn 0.107 0.269 0.839
Zn 0.769 0.393 0.661
Zn 0.607 0.769 0.661
Zn 0.393 0.231 0.661
Zn 0.231 0.607 0.661
Zn 0.769 0.607 0.339
Zn 0.607 0.231 0.339
Zn 0.393 0.769 0.339
Zn 0.231 0.393 0.339
Zn 0.893 0.269 0.161
Zn 0.731 0.893 0.161
Zn 0.269 0.107 0.161
Zn 0.107 0.731 0.161
O 0.893 0.266 0.836
O 0.734 0.893 0.836
O 0.266 0.107 0.836
O 0.107 0.734 0.836
O 0.766 0.607 0.664
O 0.607 0.234 0.664
O 0.393 0.766 0.664
O 0.234 0.393 0.664
O 0.766 0.393 0.336
O 0.607 0.766 0.336
O 0.393 0.234 0.336
O 0.234 0.607 0.336
O 0.893 0.734 0.164
O 0.734 0.107 0.164
O 0.266 0.893 0.164
O 0.107 0.266 0.164

Str 68 (UMK)[19]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.85 eV
E_{rel}: 0.24 eV/ZnO
$Pore_{max}$: 0.48 nm
V_{pore}: 22 %
D_{pore}: 1
cell parameters
8.947 8.948 5.559 90.00 90.00 120.00
fractional coordinates

Zn 0.321 0.451 0.934
Zn 0.127 0.668 0.934
Zn 0.538 0.862 0.934
Zn 0.864 0.536 0.570
Zn 0.669 0.125 0.570
Zn 0.453 0.320 0.570
Zn 0.127 0.451 0.434
Zn 0.538 0.668 0.434
Zn 0.321 0.862 0.434
Zn 0.864 0.320 0.070
Zn 0.669 0.536 0.070
Zn 0.453 0.125 0.070
O 0.867 0.538 0.936
O 0.667 0.122 0.935
O 0.451 0.322 0.935
O 0.323 0.450 0.569
O 0.123 0.666 0.569
O 0.539 0.866 0.569
O 0.867 0.322 0.436
O 0.667 0.538 0.436
O 0.451 0.122 0.435
O 0.123 0.450 0.069
O 0.323 0.866 0.069
O 0.539 0.666 0.069

Str 69 (LEV)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.84 eV
E_{rel}: 0.28 eV/ZnO
$Pore_{max}$: 0.37 nm
V_{pore}: 22 %
D_{pore}: 3
cell parameters
8.203 8.203 30.509 90.00 90.00 120.00
fractional coordinates
Zn 0.755 0.758 0.966
Zn 0.242 0.997 0.966
Zn 0.003 0.245 0.966
Zn 0.915 0.582 0.917
Zn 0.667 0.085 0.917
Zn 0.418 0.333 0.917
Zn 0.578 0.669 0.867
Zn 0.331 0.909 0.867
Zn 0.091 0.422 0.867
Zn 0.575 0.912 0.800
Zn 0.336 0.425 0.800
Zn 0.088 0.664 0.800
Zn 0.752 0.752 0.750
Zn 0.248 0.000 0.750
Zn 0.000 0.248 0.750
Zn 0.912 0.575 0.700
Zn 0.664 0.088 0.700
Zn 0.425 0.336 0.700

Zn 0.909 0.331 0.633
Zn 0.669 0.578 0.633
Zn 0.422 0.091 0.633
Zn 0.582 0.915 0.583
Zn 0.333 0.418 0.583
Zn 0.085 0.667 0.583
Zn 0.997 0.242 0.534
Zn 0.758 0.755 0.534
Zn 0.245 0.003 0.534
Zn 0.755 0.997 0.466
Zn 0.242 0.245 0.466
Zn 0.003 0.758 0.466
Zn 0.915 0.333 0.417
Zn 0.667 0.582 0.417
Zn 0.418 0.085 0.417
Zn 0.578 0.909 0.367
Zn 0.331 0.422 0.367
Zn 0.091 0.669 0.367
Zn 0.575 0.664 0.300
Zn 0.336 0.912 0.300
Zn 0.088 0.425 0.300
Zn 0.752 0.000 0.250
Zn 0.248 0.248 0.250
Zn 0.000 0.752 0.250
Zn 0.912 0.336 0.200
Zn 0.664 0.575 0.200
Zn 0.425 0.088 0.200
Zn 0.909 0.578 0.133
Zn 0.669 0.091 0.133
Zn 0.422 0.331 0.133
Zn 0.582 0.667 0.083
Zn 0.333 0.915 0.083
Zn 0.085 0.418 0.083
Zn 0.997 0.755 0.034
Zn 0.758 0.003 0.034
Zn 0.245 0.242 0.034
O 0.747 0.992 0.967
O 0.246 0.253 0.967
O 0.008 0.754 0.967
O 0.912 0.333 0.917
O 0.667 0.578 0.917
O 0.422 0.088 0.917
O 0.587 0.912 0.866
O 0.326 0.413 0.866
O 0.088 0.674 0.866
O 0.579 0.659 0.800
O 0.341 0.920 0.800
O 0.080 0.421 0.800
O 0.755 0.000 0.750
O 0.245 0.245 0.750
O 0.000 0.755 0.750
O 0.920 0.341 0.700

O 0.659 0.579 0.700
O 0.421 0.080 0.700
O 0.912 0.587 0.634
O 0.674 0.088 0.634
O 0.413 0.326 0.634
O 0.578 0.667 0.583
O 0.333 0.912 0.583
O 0.088 0.422 0.583
O 0.992 0.747 0.533
O 0.754 0.008 0.533
O 0.253 0.246 0.533
O 0.747 0.754 0.467
O 0.246 0.992 0.467
O 0.008 0.253 0.467
O 0.912 0.578 0.417
O 0.667 0.088 0.417
O 0.422 0.333 0.417
O 0.587 0.674 0.366
O 0.326 0.912 0.366
O 0.088 0.413 0.366
O 0.579 0.920 0.300
O 0.341 0.421 0.300
O 0.080 0.659 0.300
O 0.755 0.755 0.250
O 0.245 0.000 0.250
O 0.000 0.245 0.250
O 0.920 0.579 0.200
O 0.659 0.080 0.200
O 0.421 0.341 0.200
O 0.912 0.326 0.134
O 0.674 0.587 0.134
O 0.413 0.088 0.134
O 0.578 0.912 0.083
O 0.333 0.422 0.083
O 0.088 0.667 0.083
O 0.992 0.246 0.033
O 0.754 0.747 0.033
O 0.253 0.008 0.033

Str 70 (EZT)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.73 eV
E_{rel}: 0.30 eV/ZnO
$Pore_{max}$: 0.38 nm
V_{pore}: 22 %
D_{pore}: 3
cell parameters
6.893 8.088 13.962 89.45 90.00 90.00
fractional coordinates
Zn 0.500 0.133 0.926
Zn 0.759 0.875 0.884
Zn 0.241 0.875 0.884
Zn 0.500 0.540 0.823

Zn 0.000 0.616 0.807
Zn 0.500 0.884 0.693
Zn 0.000 0.960 0.677
Zn 0.741 0.625 0.616
Zn 0.259 0.625 0.616
Zn 0.000 0.367 0.574
Zn 0.793 0.000 0.500
Zn 0.207 0.000 0.500
Zn 0.000 0.633 0.426
Zn 0.741 0.375 0.384
Zn 0.259 0.375 0.384
Zn 0.000 0.040 0.323
Zn 0.500 0.116 0.307
Zn 0.000 0.384 0.193
Zn 0.500 0.460 0.177
Zn 0.759 0.125 0.116
Zn 0.241 0.125 0.116
Zn 0.500 0.867 0.074
Zn 0.707 0.500 0.000
Zn 0.293 0.500 0.000
O 0.500 0.366 0.923
O 0.760 0.625 0.885
O 0.240 0.625 0.885
O 0.500 0.954 0.824
O 0.000 0.888 0.808
O 0.500 0.612 0.692
O 0.000 0.546 0.676
O 0.740 0.875 0.615
O 0.260 0.875 0.615
O 0.000 0.134 0.577
O 0.792 0.500 0.500
O 0.208 0.500 0.500
O 0.000 0.866 0.423
O 0.740 0.125 0.385
O 0.260 0.125 0.385
O 0.000 0.454 0.324
O 0.500 0.388 0.308
O 0.000 0.112 0.192
O 0.500 0.046 0.176
O 0.760 0.375 0.115
O 0.240 0.375 0.115
O 0.500 0.634 0.077
O 0.708 1.000 0.000
O 0.292 1.000 0.000

Str 71 (EAB)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.73 eV
E_{rel}: 0.28 eV/ZnO
$Pore_{max}$: 0.37 nm
V_{pore}: 22 %
D_{pore}: 3
cell parameters

8.196 8.196 10.188 90.00 90.00 120.00
fractional coordinates
Zn 0.575 0.912 0.851
Zn 0.337 0.425 0.851
Zn 0.088 0.663 0.851
Zn 0.575 0.663 0.649
Zn 0.337 0.912 0.649
Zn 0.088 0.425 0.649
Zn 0.752 0.000 0.500
Zn 0.248 0.248 0.500
Zn 0.000 0.752 0.500
Zn 0.912 0.337 0.351
Zn 0.663 0.575 0.351
Zn 0.425 0.088 0.351
Zn 0.912 0.575 0.149
Zn 0.663 0.088 0.149
Zn 0.425 0.337 0.149
Zn 0.752 0.752 0.000
Zn 0.248 0.000 0.000
Zn 0.000 0.248 0.000
O 0.580 0.661 0.848
O 0.339 0.919 0.848
O 0.081 0.420 0.848
O 0.580 0.919 0.652
O 0.339 0.420 0.652
O 0.081 0.661 0.652
O 0.754 0.754 0.500
O 0.246 0.000 0.500
O 0.000 0.246 0.500
O 0.919 0.580 0.348
O 0.661 0.081 0.348
O 0.420 0.339 0.348
O 0.919 0.339 0.152
O 0.661 0.580 0.152
O 0.420 0.081 0.152
O 0.754 0.000 0.000
O 0.246 0.246 0.000
O 0.000 0.754 0.000

Str 72 (ATS)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.78 eV
E_{rel}: 0.23 eV/ZnO
$Pore_{max}$: 0.40 nm
V_{pore}: 22 %
D_{pore}: 1
cell parameters
8.430 13.663 3.391 90.00 90.00 89.72
fractional coordinates
Zn 0.872 0.527 0.750
Zn 0.689 0.164 0.750
Zn 0.616 0.750 0.750
Zn 0.372 0.027 0.750

Zn 0.189 0.664 0.750
Zn 0.116 0.250 0.750
Zn 0.889 0.731 0.250
Zn 0.815 0.317 0.250
Zn 0.633 0.954 0.250
Zn 0.389 0.231 0.250
Zn 0.315 0.817 0.250
Zn 0.133 0.454 0.250
O 0.888 0.248 0.750
O 0.810 0.663 0.750
O 0.634 0.028 0.750
O 0.388 0.748 0.750
O 0.310 0.163 0.750
O 0.134 0.528 0.750
O 0.695 0.818 0.250
O 0.616 0.233 0.250
O 0.370 0.954 0.250
O 0.195 0.318 0.250
O 0.116 0.733 0.250
O 0.870 0.454 0.250

Str 73 (BCB)[19]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.75 eV
E_{rel}: 0.27 eV/ZnO
$Pore_{max}$: 0.47 nm
V_{pore}: 23 %
D_{pore}: 3
cell parameters
8.825 8.827 3.400 90.00 90.00 90.03
fractional coordinates
Zn 0.787 0.656 0.574
Zn 0.636 0.245 0.574
Zn 0.376 0.806 0.574
Zn 0.226 0.396 0.574
Zn 0.894 0.410 0.074
Zn 0.622 0.913 0.074
Zn 0.391 0.139 0.074
Zn 0.119 0.641 0.074
O 0.779 0.414 0.574
O 0.619 0.798 0.574
O 0.394 0.253 0.574
O 0.234 0.638 0.574
O 0.900 0.662 0.074
O 0.642 0.132 0.074
O 0.371 0.920 0.074
O 0.113 0.390 0.074

Str 74 (LTL)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.73 eV
E_{rel}: 0.33 eV/ZnO
$Pore_{max}$: 0.65 nm
V_{pore}: 24 %

D_{pore}: 3
cell parameters
11.418 11.418 10.623 90.00 90.00 120.00
fractional coordinates
Zn 0.844 0.335 0.903
Zn 0.665 0.509 0.903
Zn 0.509 0.844 0.903
Zn 0.491 0.156 0.903
Zn 0.335 0.491 0.903
Zn 0.156 0.665 0.903
Zn 0.905 0.624 0.750
Zn 0.718 0.095 0.750
Zn 0.624 0.718 0.750
Zn 0.376 0.282 0.750
Zn 0.282 0.905 0.750
Zn 0.095 0.376 0.750
Zn 0.844 0.335 0.597
Zn 0.665 0.509 0.597
Zn 0.509 0.844 0.597
Zn 0.491 0.156 0.597
Zn 0.335 0.491 0.597
Zn 0.156 0.665 0.597
Zn 0.844 0.509 0.403
Zn 0.665 0.156 0.403
Zn 0.509 0.665 0.403
Zn 0.491 0.335 0.403
Zn 0.335 0.844 0.403
Zn 0.156 0.491 0.403
Zn 0.905 0.282 0.250
Zn 0.718 0.624 0.250
Zn 0.624 0.905 0.250
Zn 0.376 0.095 0.250
Zn 0.282 0.376 0.250
Zn 0.095 0.718 0.250
Zn 0.844 0.509 0.097
Zn 0.665 0.156 0.097
Zn 0.509 0.665 0.097
Zn 0.491 0.335 0.097
Zn 0.335 0.844 0.097
Zn 0.156 0.491 0.097
O 0.849 0.511 0.906
O 0.662 0.151 0.906
O 0.511 0.662 0.906
O 0.489 0.338 0.906
O 0.338 0.849 0.906
O 0.151 0.489 0.906
O 0.899 0.272 0.750
O 0.728 0.627 0.750
O 0.627 0.899 0.750
O 0.373 0.101 0.750
O 0.272 0.373 0.750
O 0.101 0.728 0.750

O 0.849 0.511 0.594
O 0.662 0.151 0.594
O 0.511 0.662 0.594
O 0.489 0.338 0.594
O 0.338 0.849 0.594
O 0.151 0.489 0.594
O 0.849 0.338 0.406
O 0.662 0.511 0.406
O 0.511 0.849 0.406
O 0.489 0.151 0.406
O 0.338 0.489 0.406
O 0.151 0.662 0.406
O 0.899 0.627 0.250
O 0.728 0.101 0.250
O 0.627 0.728 0.250
O 0.373 0.272 0.250
O 0.272 0.899 0.250
O 0.101 0.373 0.250
O 0.849 0.338 0.094
O 0.662 0.511 0.094
O 0.511 0.849 0.094
O 0.489 0.151 0.094
O 0.338 0.489 0.094
O 0.151 0.662 0.094

Str 75 (VFI)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.71 eV
E_{rel}: 0.28 eV/ZnO
$Pore_{max}$: 0.57 nm
V_{pore}: 25 %
D_{pore}: 1
cell parameters
11.552 11.552 5.372 90.00 90.00 120.01
fractional coordinates
Zn 1.000 0.377 0.583
Zn 0.377 1.000 0.583
Zn 0.623 0.623 0.583
Zn 0.674 0.168 0.560
Zn 0.168 0.674 0.560
Zn 0.506 0.832 0.560
Zn 0.494 0.326 0.560
Zn 0.326 0.494 0.560
Zn 0.832 0.506 0.560
Zn 0.623 0.000 0.083
Zn 0.000 0.623 0.083
Zn 0.377 0.377 0.083
Zn 0.832 0.326 0.060
Zn 0.494 0.168 0.060
Zn 0.326 0.832 0.060
Zn 0.168 0.494 0.060
Zn 0.674 0.506 0.060
Zn 0.506 0.674 0.060

O 0.666 0.170 0.933
O 0.504 0.334 0.933
O 0.496 0.830 0.933
O 0.334 0.504 0.933
O 0.170 0.666 0.933
O 0.830 0.496 0.933
O 1.000 0.351 0.930
O 0.351 1.000 0.930
O 0.649 0.649 0.930
O 0.830 0.334 0.433
O 0.504 0.170 0.433
O 0.334 0.830 0.433
O 0.170 0.504 0.433
O 0.666 0.496 0.433
O 0.496 0.666 0.433
O 0.649 0.000 0.430
O 0.000 0.649 0.430
O 0.351 0.351 0.430

Str 76 (CHA)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 1.21 eV
E_{rel}: 0.30 eV/ZnO
$Pore_{max}$: 0.39 nm
V_{pore}: 26 %
D_{pore}: 3
cell parameters
8.575 8.577 9.857 90.00 90.00 120.00
fractional coordinates
Zn 0.566 0.919 0.962
Zn 0.092 0.672 0.962
Zn 0.340 0.446 0.962
Zn 0.326 0.912 0.752
Zn 0.573 0.686 0.752
Zn 0.099 0.439 0.752
Zn 0.899 0.586 0.629
Zn 0.673 0.112 0.629
Zn 0.426 0.339 0.629
Zn 0.907 0.353 0.419
Zn 0.659 0.579 0.419
Zn 0.433 0.105 0.419
Zn 0.007 0.779 0.296
Zn 0.759 0.005 0.295
Zn 0.233 0.253 0.295
Zn 0.992 0.246 0.086
Zn 0.240 0.019 0.086
Zn 0.766 0.772 0.086
O 0.093 0.446 0.961
O 0.566 0.673 0.961
O 0.339 0.919 0.961
O 0.100 0.685 0.753
O 0.573 0.912 0.753
O 0.326 0.439 0.753

O 0.899 0.339 0.628
O 0.426 0.112 0.628
O 0.672 0.585 0.627
O 0.906 0.579 0.420
O 0.660 0.106 0.420
O 0.433 0.352 0.420
O 0.233 0.006 0.294
O 0.006 0.252 0.294
O 0.760 0.779 0.294
O 0.993 0.773 0.087
O 0.766 0.019 0.087
O 0.239 0.246 0.087

Str 77 (GME)[17]
ΔE_{gap}(PBE$_{GW-fit}$): 1.07 eV
E_{rel}: 0.29 eV/ZnO
Pore$_{max}$: 0.43 nm
V_{pore}: 26 %
D_{pore}: 3
cell parameters
8.670 8.670 6.440 90.00 90.00 120.00
fractional coordinates
Zn 0.571 0.673 0.910
Zn 0.327 0.898 0.910
Zn 0.102 0.429 0.910
Zn 0.571 0.898 0.590
Zn 0.327 0.429 0.590
Zn 0.102 0.673 0.590
Zn 0.898 0.327 0.410
Zn 0.673 0.571 0.410
Zn 0.429 0.102 0.410
Zn 0.898 0.571 0.090
Zn 0.673 0.102 0.090
Zn 0.429 0.327 0.090
O 0.569 0.896 0.910
O 0.327 0.431 0.910
O 0.104 0.673 0.910
O 0.569 0.673 0.590
O 0.327 0.896 0.590
O 0.104 0.431 0.590
O 0.896 0.569 0.410
O 0.673 0.104 0.410
O 0.431 0.327 0.410
O 0.896 0.327 0.090
O 0.673 0.569 0.090
O 0.431 0.104 0.090

Str 78 (AFR)[17]
ΔE_{gap}(PBE$_{GW-fit}$): 1.04 eV
E_{rel}: 0.34 eV/ZnO
Pore$_{max}$: 0.48 nm
V_{pore}: 28 %

D_{pore}: 2
cell parameters
14.284 8.771 9.083 90.00 90.00 90.00
fractional coordinates
Zn 0.816 0.622 0.938
Zn 0.684 0.878 0.938
Zn 0.483 0.860 0.923
Zn 0.017 0.640 0.923
Zn 0.412 0.454 0.922
Zn 0.088 0.046 0.922
Zn 0.909 0.862 0.773
Zn 0.591 0.638 0.773
Zn 0.409 0.138 0.727
Zn 0.091 0.362 0.727
Zn 0.912 0.546 0.578
Zn 0.588 0.954 0.578
Zn 0.983 0.140 0.577
Zn 0.517 0.360 0.577
Zn 0.316 0.378 0.562
Zn 0.184 0.122 0.562
Zn 0.816 0.878 0.438
Zn 0.684 0.622 0.438
Zn 0.483 0.640 0.423
Zn 0.017 0.860 0.423
Zn 0.412 0.046 0.422
Zn 0.088 0.454 0.422
Zn 0.909 0.638 0.273
Zn 0.591 0.862 0.273
Zn 0.409 0.362 0.227
Zn 0.091 0.138 0.227
Zn 0.912 0.954 0.078
Zn 0.588 0.546 0.078
Zn 0.983 0.360 0.077
Zn 0.517 0.140 0.077
Zn 0.316 0.122 0.062
Zn 0.184 0.378 0.062
O 0.817 0.879 0.940
O 0.683 0.621 0.940
O 0.486 0.642 0.929
O 0.014 0.858 0.929
O 0.412 0.048 0.920
O 0.088 0.452 0.920
O 0.907 0.630 0.774
O 0.592 0.870 0.774
O 0.407 0.370 0.726
O 0.092 0.130 0.726
O 0.912 0.952 0.580
O 0.588 0.548 0.580
O 0.986 0.358 0.571
O 0.514 0.142 0.571
O 0.317 0.121 0.560
O 0.183 0.379 0.560

O 0.817 0.621 0.440
O 0.683 0.879 0.440
O 0.486 0.858 0.429
O 0.014 0.642 0.429
O 0.412 0.452 0.420
O 0.088 0.048 0.420
O 0.907 0.870 0.274
O 0.592 0.630 0.274
O 0.407 0.130 0.226
O 0.092 0.370 0.226
O 0.912 0.548 0.080
O 0.588 0.952 0.080
O 0.986 0.142 0.071
O 0.514 0.358 0.071
O 0.317 0.379 0.060
O 0.183 0.121 0.060

Str 79 (SFO)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 1.03 eV
E_{rel}: 0.34 eV/ZnO
$Pore_{max}$: 0.47 nm
V_{pore}: 28 %
D_{pore}: 2
cell parameters
14.435 8.766 9.091 90.00 98.36 90.00
fractional coordinates
Zn 0.934 0.873 0.980
Zn 0.434 0.373 0.980
Zn 0.733 0.890 0.919
Zn 0.233 0.390 0.919
Zn 0.662 0.297 0.903
Zn 0.162 0.797 0.903
Zn 0.341 0.612 0.793
Zn 0.841 0.112 0.793
Zn 0.659 0.612 0.707
Zn 0.159 0.112 0.707
Zn 0.838 0.797 0.597
Zn 0.338 0.297 0.597
Zn 0.767 0.390 0.581
Zn 0.267 0.890 0.581
Zn 0.566 0.373 0.520
Zn 0.066 0.873 0.520
Zn 0.934 0.127 0.480
Zn 0.434 0.627 0.480
Zn 0.733 0.110 0.419
Zn 0.233 0.610 0.419
Zn 0.662 0.703 0.403
Zn 0.162 0.203 0.403
Zn 0.841 0.888 0.293
Zn 0.341 0.388 0.293
Zn 0.659 0.388 0.207
Zn 0.159 0.888 0.207

Zn 0.838 0.203 0.097
Zn 0.338 0.703 0.097
Zn 0.767 0.610 0.081
Zn 0.267 0.110 0.081
Zn 0.566 0.627 0.020
Zn 0.066 0.127 0.020
O 0.933 0.129 0.981
O 0.433 0.629 0.981
O 0.736 0.108 0.925
O 0.236 0.608 0.925
O 0.663 0.702 0.900
O 0.163 0.202 0.900
O 0.843 0.880 0.795
O 0.343 0.380 0.795
O 0.657 0.380 0.705
O 0.157 0.880 0.705
O 0.837 0.202 0.600
O 0.337 0.702 0.600
O 0.764 0.608 0.575
O 0.264 0.108 0.575
O 0.567 0.629 0.519
O 0.067 0.129 0.519
O 0.933 0.871 0.481
O 0.433 0.371 0.481
O 0.736 0.892 0.425
O 0.236 0.392 0.425
O 0.663 0.298 0.400
O 0.163 0.798 0.400
O 0.843 0.120 0.295
O 0.343 0.620 0.295
O 0.657 0.620 0.205
O 0.157 0.120 0.205
O 0.837 0.798 0.100
O 0.337 0.298 0.100
O 0.764 0.392 0.075
O 0.264 0.892 0.075
O 0.567 0.371 0.019
O 0.067 0.871 0.019

Str 80 (USI)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 0.77 eV
E_{rel}: 0.44 eV/ZnO
$Pore_{max}$: 0.42 nm
V_{pore}: 29 %
D_{pore}: 2
cell parameters
13.825 8.406 6.433 90.00 108.75 90.15
fractional coordinates
Zn 0.286 0.118 0.896
Zn 0.786 0.618 0.896
Zn 0.689 0.177 0.801
Zn 0.189 0.677 0.801

Zn 0.841 0.329 0.653
Zn 0.341 0.829 0.653
Zn 0.785 0.886 0.635
Zn 0.285 0.386 0.635
Zn 0.072 0.368 0.535
Zn 0.572 0.868 0.535
Zn 0.928 0.632 0.465
Zn 0.428 0.132 0.465
Zn 0.715 0.614 0.365
Zn 0.215 0.114 0.365
Zn 0.659 0.171 0.347
Zn 0.159 0.671 0.347
Zn 0.811 0.323 0.199
Zn 0.311 0.823 0.199
Zn 0.214 0.382 0.104
Zn 0.714 0.882 0.104
O 0.785 0.382 0.892
O 0.285 0.882 0.892
O 0.183 0.306 0.800
O 0.683 0.806 0.800
O 0.847 0.678 0.663
O 0.347 0.178 0.663
O 0.785 0.108 0.633
O 0.285 0.608 0.633
O 0.573 0.129 0.531
O 0.073 0.629 0.531
O 0.927 0.371 0.469
O 0.427 0.871 0.469
O 0.715 0.392 0.367
O 0.215 0.892 0.367
O 0.153 0.322 0.337
O 0.653 0.822 0.337
O 0.817 0.694 0.200
O 0.317 0.194 0.200
O 0.715 0.118 0.108
O 0.215 0.618 0.108

Str 81 (LTA)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 1.43 eV
E_{rel}: 0.25 eV/ZnO
$Pore_{max}$: 0.64 nm
V_{pore}: 30 %
D_{pore}: 3
cell parameters
10.759 10.759 10.759 60.00 60.00 60.00
fractional coordinates
Zn 0.719 0.281 0.914
Zn 0.281 0.086 0.914
Zn 0.086 0.719 0.914
Zn 0.586 0.219 0.781
Zn 0.414 0.586 0.781
Zn 0.219 0.414 0.781

Zn 0.914 0.086 0.719
Zn 0.281 0.914 0.719
Zn 0.086 0.281 0.719
Zn 0.781 0.414 0.586
Zn 0.414 0.219 0.586
Zn 0.219 0.781 0.586
Zn 0.781 0.219 0.414
Zn 0.586 0.781 0.414
Zn 0.219 0.586 0.414
Zn 0.914 0.719 0.281
Zn 0.719 0.086 0.281
Zn 0.086 0.914 0.281
Zn 0.781 0.586 0.219
Zn 0.586 0.414 0.219
Zn 0.414 0.781 0.219
Zn 0.914 0.281 0.086
Zn 0.719 0.914 0.086
Zn 0.281 0.719 0.086
O 0.720 0.089 0.911
O 0.280 0.720 0.911
O 0.089 0.280 0.911
O 0.589 0.411 0.780
O 0.411 0.220 0.780
O 0.220 0.589 0.780
O 0.911 0.280 0.720
O 0.280 0.089 0.720
O 0.089 0.911 0.720
O 0.780 0.220 0.589
O 0.411 0.780 0.589
O 0.220 0.411 0.589
O 0.780 0.589 0.411
O 0.589 0.220 0.411
O 0.220 0.780 0.411
O 0.911 0.089 0.280
O 0.720 0.911 0.280
O 0.089 0.720 0.280
O 0.780 0.411 0.220
O 0.589 0.780 0.220
O 0.411 0.589 0.220
O 0.911 0.720 0.089
O 0.720 0.280 0.089
O 0.280 0.911 0.089

Str 82 (AFS)[17]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 1.22 eV
E_{rel}: 0.36 eV/ZnO
$Pore_{max}$: 0.56 nm
V_{pore}: 31 %
D_{pore}: 3
cell parameters
8.526 8.526 16.493 90.00 90.00 120.00
fractional coordinates

```
Zn 0.667 0.333 0.945
Zn 0.517 0.645 0.868
Zn 0.355 0.872 0.868
Zn 0.128 0.483 0.868
Zn 0.864 0.574 0.811
Zn 0.710 0.136 0.811
Zn 0.426 0.290 0.811
Zn 0.574 0.864 0.689
Zn 0.290 0.426 0.689
Zn 0.136 0.710 0.689
Zn 0.872 0.355 0.632
Zn 0.645 0.517 0.632
Zn 0.483 0.128 0.632
Zn 0.333 0.667 0.555
Zn 0.667 0.333 0.445
Zn 0.517 0.872 0.368
Zn 0.355 0.483 0.368
Zn 0.128 0.645 0.368
Zn 0.864 0.290 0.311
Zn 0.710 0.574 0.311
Zn 0.426 0.136 0.311
Zn 0.574 0.710 0.189
Zn 0.290 0.864 0.189
Zn 0.136 0.426 0.189
Zn 0.872 0.517 0.132
Zn 0.645 0.128 0.132
Zn 0.483 0.355 0.132
Zn 0.333 0.667 0.055
O 0.333 0.667 0.940
O 0.869 0.349 0.873
O 0.651 0.520 0.873
O 0.480 0.131 0.873
O 0.576 0.867 0.810
O 0.291 0.424 0.810
O 0.133 0.709 0.810
O 0.867 0.576 0.690
O 0.709 0.133 0.690
O 0.424 0.291 0.690
O 0.520 0.651 0.627
O 0.349 0.869 0.627
O 0.131 0.480 0.627
O 0.667 0.333 0.560
O 0.333 0.667 0.440
O 0.869 0.520 0.373
O 0.651 0.131 0.373
O 0.480 0.349 0.373
O 0.576 0.709 0.310
O 0.291 0.867 0.310
O 0.133 0.424 0.310
O 0.867 0.291 0.190
O 0.709 0.576 0.190
O 0.424 0.133 0.190
```

O 0.520 0.869 0.127
O 0.349 0.480 0.127
O 0.131 0.651 0.127
O 0.667 0.333 0.060

Str 83 (SAO)[17]
$\Delta E_{gap}(PBE_{GW-fit})$: 1.18 eV
E_{rel}: 0.38 eV/ZnO
$Pore_{max}$: 0.49 nm
V_{pore}: 34 %
D_{pore}: 3
cell parameters
8.925 8.925 13.591 90.00 90.00 90.00
fractional coordinates
Zn 0.606 0.877 0.948
Zn 0.394 0.123 0.948
Zn 0.896 0.878 0.874
Zn 0.104 0.122 0.874
Zn 0.700 0.117 0.807
Zn 0.300 0.883 0.807
Zn 0.617 0.800 0.693
Zn 0.383 0.200 0.693
Zn 0.622 0.396 0.626
Zn 0.378 0.604 0.626
Zn 0.623 0.106 0.552
Zn 0.377 0.894 0.552
Zn 0.704 0.704 0.500
Zn 0.296 0.296 0.500
Zn 0.894 0.377 0.448
Zn 0.106 0.623 0.448
Zn 0.604 0.378 0.374
Zn 0.396 0.622 0.374
Zn 0.800 0.617 0.307
Zn 0.200 0.383 0.307
Zn 0.883 0.300 0.193
Zn 0.117 0.700 0.193
Zn 0.878 0.896 0.126
Zn 0.122 0.104 0.126
Zn 0.877 0.606 0.052
Zn 0.123 0.394 0.052
Zn 0.796 0.204 0.000
Zn 0.204 0.796 0.000
O 0.607 0.121 0.947
O 0.393 0.879 0.947
O 0.894 0.127 0.876
O 0.106 0.873 0.876
O 0.703 0.885 0.807
O 0.297 0.115 0.807
O 0.615 0.203 0.693
O 0.385 0.797 0.693
O 0.627 0.606 0.624
O 0.373 0.394 0.624

O 0.621 0.893 0.553
O 0.379 0.107 0.553
O 0.704 0.296 0.500
O 0.296 0.704 0.500
O 0.893 0.621 0.447
O 0.107 0.379 0.447
O 0.606 0.627 0.376
O 0.394 0.373 0.376
O 0.797 0.385 0.307
O 0.203 0.615 0.307
O 0.885 0.703 0.193
O 0.115 0.297 0.193
O 0.873 0.106 0.124
O 0.127 0.894 0.124
O 0.879 0.393 0.053
O 0.121 0.607 0.053
O 0.796 0.796 0.000
O 0.204 0.204 0.000

Str 84 (BBZ)[19]
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.83 eV
E_{rel}: 0.25 eV/ZnO
$Pore_{max}$: 0.84 nm
V_{pore}: 36 %
D_{pore}: 3
cell parameters
12.902 12.901 3.370 90.00 90.00 120.01
fractional coordinates
Zn 0.822 0.334 0.500
Zn 0.673 0.512 0.500
Zn 0.498 0.836 0.500
Zn 0.495 0.185 0.500
Zn 0.320 0.509 0.500
Zn 0.172 0.687 0.500
Zn 0.909 0.548 0.000
Zn 0.622 0.099 0.000
Zn 0.534 0.636 0.000
Zn 0.460 0.386 0.000
Zn 0.372 0.923 0.000
Zn 0.085 0.474 0.000
O 0.819 0.503 0.500
O 0.667 0.189 0.500
O 0.504 0.340 0.500
O 0.489 0.681 0.500
O 0.326 0.832 0.500
O 0.175 0.518 0.500
O 0.912 0.375 0.000
O 0.632 0.561 0.000
O 0.547 0.926 0.000
O 0.447 0.096 0.000
O 0.362 0.461 0.000
O 0.082 0.646 0.000

Str 85 (FAU)[17]

$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 1.16 eV

E_{rel}: 0.34 eV/ZnO

$Pore_{max}$: 0.67 nm

V_{pore}: 38 %

D_{pore}: 3

cell parameters

15.834 15.834 15.834 90.00 90.00 90.00

fractional coordinates

Zn 0.880 0.196 0.965
Zn 0.870 0.554 0.965
Zn 0.380 0.696 0.965
Zn 0.370 0.054 0.965
Zn 0.715 0.120 0.946
Zn 0.535 0.130 0.946
Zn 0.215 0.620 0.946
Zn 0.035 0.630 0.946
Zn 0.696 0.465 0.880
Zn 0.554 0.785 0.880
Zn 0.196 0.965 0.880
Zn 0.054 0.285 0.880
Zn 0.696 0.285 0.870
Zn 0.554 0.965 0.870
Zn 0.196 0.785 0.870
Zn 0.054 0.465 0.870
Zn 0.715 0.630 0.804
Zn 0.535 0.620 0.804
Zn 0.215 0.130 0.804
Zn 0.035 0.120 0.804
Zn 0.880 0.554 0.785
Zn 0.870 0.196 0.785
Zn 0.380 0.054 0.785
Zn 0.370 0.696 0.785
Zn 0.630 0.804 0.715
Zn 0.620 0.446 0.715
Zn 0.130 0.304 0.715
Zn 0.120 0.946 0.715
Zn 0.965 0.380 0.696
Zn 0.785 0.370 0.696
Zn 0.465 0.880 0.696
Zn 0.285 0.870 0.696
Zn 0.946 0.035 0.630
Zn 0.804 0.715 0.630
Zn 0.446 0.535 0.630
Zn 0.304 0.215 0.630
Zn 0.946 0.215 0.620
Zn 0.804 0.535 0.620
Zn 0.446 0.715 0.620
Zn 0.304 0.035 0.620
Zn 0.965 0.870 0.554
Zn 0.785 0.880 0.554

Zn 0.465 0.370 0.554
Zn 0.285 0.380 0.554
Zn 0.630 0.446 0.535
Zn 0.620 0.804 0.535
Zn 0.130 0.946 0.535
Zn 0.120 0.304 0.535
Zn 0.880 0.696 0.465
Zn 0.870 0.054 0.465
Zn 0.380 0.196 0.465
Zn 0.370 0.554 0.465
Zn 0.715 0.620 0.446
Zn 0.535 0.630 0.446
Zn 0.215 0.120 0.446
Zn 0.035 0.130 0.446
Zn 0.696 0.965 0.380
Zn 0.554 0.285 0.380
Zn 0.196 0.465 0.380
Zn 0.054 0.785 0.380
Zn 0.696 0.785 0.370
Zn 0.554 0.465 0.370
Zn 0.196 0.285 0.370
Zn 0.054 0.965 0.370
Zn 0.715 0.130 0.304
Zn 0.535 0.120 0.304
Zn 0.215 0.630 0.304
Zn 0.035 0.620 0.304
Zn 0.880 0.054 0.285
Zn 0.870 0.696 0.285
Zn 0.380 0.554 0.285
Zn 0.370 0.196 0.285
Zn 0.630 0.304 0.215
Zn 0.620 0.946 0.215
Zn 0.130 0.804 0.215
Zn 0.120 0.446 0.215
Zn 0.965 0.880 0.196
Zn 0.785 0.870 0.196
Zn 0.465 0.380 0.196
Zn 0.285 0.370 0.196
Zn 0.946 0.535 0.130
Zn 0.804 0.215 0.130
Zn 0.446 0.035 0.130
Zn 0.304 0.715 0.130
Zn 0.946 0.715 0.120
Zn 0.804 0.035 0.120
Zn 0.446 0.215 0.120
Zn 0.304 0.535 0.120
Zn 0.965 0.370 0.054
Zn 0.785 0.380 0.054
Zn 0.465 0.870 0.054
Zn 0.285 0.880 0.054
Zn 0.630 0.946 0.035
Zn 0.620 0.304 0.035

Zn 0.130 0.446 0.035
Zn 0.120 0.804 0.035
O 0.695 0.380 0.966
O 0.555 0.870 0.966
O 0.195 0.880 0.966
O 0.055 0.370 0.966
O 0.630 0.034 0.945
O 0.620 0.216 0.945
O 0.130 0.534 0.945
O 0.120 0.716 0.945
O 0.966 0.195 0.880
O 0.784 0.555 0.880
O 0.466 0.695 0.880
O 0.284 0.055 0.880
O 0.966 0.555 0.870
O 0.784 0.195 0.870
O 0.466 0.055 0.870
O 0.284 0.695 0.870
O 0.630 0.716 0.805
O 0.620 0.534 0.805
O 0.130 0.216 0.805
O 0.120 0.034 0.805
O 0.695 0.370 0.784
O 0.555 0.880 0.784
O 0.195 0.870 0.784
O 0.055 0.380 0.784
O 0.945 0.120 0.716
O 0.805 0.630 0.716
O 0.445 0.620 0.716
O 0.305 0.130 0.716
O 0.880 0.466 0.695
O 0.870 0.284 0.695
O 0.380 0.966 0.695
O 0.370 0.784 0.695
O 0.716 0.805 0.630
O 0.534 0.445 0.630
O 0.216 0.305 0.630
O 0.034 0.945 0.630
O 0.716 0.445 0.620
O 0.534 0.805 0.620
O 0.216 0.945 0.620
O 0.034 0.305 0.620
O 0.880 0.784 0.555
O 0.870 0.966 0.555
O 0.380 0.284 0.555
O 0.370 0.466 0.555
O 0.945 0.130 0.534
O 0.805 0.620 0.534
O 0.445 0.630 0.534
O 0.305 0.120 0.534
O 0.695 0.880 0.466
O 0.555 0.370 0.466

O 0.195 0.380 0.466
O 0.055 0.870 0.466
O 0.630 0.534 0.445
O 0.620 0.716 0.445
O 0.130 0.034 0.445
O 0.120 0.216 0.445
O 0.966 0.695 0.380
O 0.784 0.055 0.380
O 0.466 0.195 0.380
O 0.284 0.555 0.380
O 0.966 0.055 0.370
O 0.784 0.695 0.370
O 0.466 0.555 0.370
O 0.284 0.195 0.370
O 0.630 0.216 0.305
O 0.620 0.034 0.305
O 0.130 0.716 0.305
O 0.120 0.534 0.305
O 0.695 0.870 0.284
O 0.555 0.380 0.284
O 0.195 0.370 0.284
O 0.055 0.880 0.284
O 0.945 0.620 0.216
O 0.805 0.130 0.216
O 0.445 0.120 0.216
O 0.305 0.630 0.216
O 0.880 0.966 0.195
O 0.870 0.784 0.195
O 0.380 0.466 0.195
O 0.370 0.284 0.195
O 0.716 0.305 0.130
O 0.534 0.945 0.130
O 0.216 0.805 0.130
O 0.034 0.445 0.130
O 0.716 0.945 0.120
O 0.534 0.305 0.120
O 0.216 0.445 0.120
O 0.034 0.805 0.120
O 0.880 0.284 0.055
O 0.870 0.466 0.055
O 0.380 0.784 0.055
O 0.370 0.966 0.055
O 0.945 0.630 0.034
O 0.805 0.120 0.034
O 0.445 0.130 0.034
O 0.305 0.620 0.034

Str 86 (EMT)[17]
ΔE_{gap}(PBE$_{GW-fit}$): 1.16 eV
E_{rel}: 0.34 eV/ZnO
Pore$_{max}$: 0.69 nm
V_{pore}: 38 %

D_{pore}: 3
cell parameters
11.201 11.201 18.270 89.99 90.00 120.00
fractional coordinates
Zn 0.261 0.213 0.945
Zn 0.799 0.561 0.945
Zn 0.451 0.751 0.945
Zn 0.345 0.015 0.911
Zn 0.168 0.667 0.911
Zn 0.998 0.844 0.911
Zn 0.569 0.272 0.857
Zn 0.202 0.443 0.857
Zn 0.740 0.810 0.857
Zn 0.105 0.078 0.816
Zn 0.472 0.907 0.816
Zn 0.934 0.540 0.816
Zn 0.329 0.335 0.762
Zn 0.677 0.506 0.762
Zn 0.506 0.683 0.762
Zn 0.413 0.137 0.727
Zn 0.223 0.599 0.727
Zn 0.875 0.789 0.727
Zn 0.167 0.023 0.642
Zn 0.355 0.845 0.642
Zn 0.989 0.657 0.642
Zn 0.355 0.023 0.531
Zn 0.168 0.657 0.531
Zn 0.989 0.845 0.531
Zn 0.224 0.138 0.445
Zn 0.414 0.789 0.445
Zn 0.875 0.599 0.445
Zn 0.329 0.507 0.410
Zn 0.506 0.336 0.410
Zn 0.677 0.684 0.410
Zn 0.472 0.078 0.357
Zn 0.106 0.541 0.357
Zn 0.934 0.907 0.357
Zn 0.202 0.272 0.316
Zn 0.741 0.443 0.316
Zn 0.570 0.811 0.316
Zn 0.169 0.015 0.262
Zn 0.998 0.667 0.262
Zn 0.346 0.844 0.262
Zn 0.451 0.213 0.227
Zn 0.261 0.561 0.227
Zn 0.800 0.751 0.227
Zn 0.319 0.327 0.142
Zn 0.507 0.693 0.142
Zn 0.686 0.505 0.142
Zn 0.507 0.327 0.031
Zn 0.319 0.505 0.031
Zn 0.685 0.693 0.031

O 0.451 0.211 0.946
O 0.259 0.561 0.945
O 0.801 0.753 0.945
O 0.169 0.016 0.912
O 0.346 0.843 0.912
O 0.996 0.666 0.912
O 0.200 0.269 0.857
O 0.743 0.443 0.857
O 0.569 0.813 0.857
O 0.474 0.080 0.816
O 0.105 0.538 0.816
O 0.932 0.907 0.816
O 0.329 0.507 0.761
O 0.505 0.334 0.761
O 0.678 0.683 0.761
O 0.223 0.139 0.727
O 0.415 0.789 0.727
O 0.873 0.597 0.727
O 0.357 0.023 0.641
O 0.165 0.655 0.641
O 0.989 0.847 0.641
O 0.165 0.023 0.532
O 0.357 0.847 0.532
O 0.990 0.655 0.532
O 0.416 0.140 0.445
O 0.224 0.597 0.445
O 0.873 0.789 0.445
O 0.329 0.335 0.412
O 0.505 0.684 0.412
O 0.678 0.508 0.411
O 0.105 0.081 0.357
O 0.475 0.908 0.357
O 0.933 0.538 0.357
O 0.570 0.270 0.316
O 0.200 0.443 0.316
O 0.743 0.813 0.315
O 0.346 0.016 0.261
O 0.997 0.843 0.261
O 0.170 0.667 0.261
O 0.259 0.211 0.227
O 0.452 0.754 0.227
O 0.802 0.561 0.227
O 0.318 0.503 0.141
O 0.509 0.327 0.141
O 0.685 0.695 0.141
O 0.317 0.327 0.032
O 0.509 0.695 0.032
O 0.685 0.503 0.032

Str 87 (WZ-ZnO-NP-1)
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.21 eV
E_{rel}: 0.08 eV/ZnO

Pore$_{max}$: 0.53 nm
V$_{pore}$: 7 %
D$_{pore}$: 1
cell parameters
19.702 19.702 5.309 90.00 90.00 120.00
fractional coordinates
Zn 0.889 0.111 0.999
Zn 0.722 0.945 0.999
Zn 0.889 0.444 0.999
Zn 0.722 0.444 0.999
Zn 0.389 0.945 0.999
Zn 0.389 0.111 0.999
Zn 0.890 0.278 0.999
Zn 0.555 0.943 0.999
Zn 0.555 0.278 0.999
Zn 0.553 0.775 0.998
Zn 0.553 0.444 0.998
Zn 0.389 0.775 0.998
Zn 0.389 0.281 0.998
Zn 0.058 0.444 0.998
Zn 0.058 0.281 0.998
Zn 0.455 0.743 0.526
Zn 0.455 0.379 0.526
Zn 0.091 0.379 0.526
Zn 0.778 0.222 0.501
Zn 0.611 0.222 0.501
Zn 0.611 0.055 0.501
Zn 0.778 0.389 0.501
Zn 0.778 0.056 0.501
Zn 0.445 0.056 0.501
Zn 0.945 0.889 0.501
Zn 0.945 0.722 0.501
Zn 0.111 0.889 0.501
Zn 0.943 0.389 0.501
Zn 0.943 0.220 0.501
Zn 0.613 0.891 0.501
Zn 0.613 0.389 0.501
Zn 0.444 0.891 0.501
Zn 0.444 0.220 0.501
Zn 0.945 0.556 0.499
Zn 0.945 0.055 0.499
Zn 0.778 0.556 0.499
Zn 0.778 0.889 0.499
Zn 0.277 0.889 0.499
Zn 0.277 0.055 0.499
Zn 0.777 0.722 0.499
Zn 0.112 0.722 0.499
Zn 0.112 0.057 0.499
Zn 0.609 0.719 0.498
Zn 0.609 0.556 0.498
Zn 0.277 0.719 0.498
Zn 0.277 0.225 0.498

Zn 0.114 0.556 0.498
Zn 0.114 0.225 0.498
Zn 0.212 0.621 0.026
Zn 0.212 0.257 0.026
Zn 0.576 0.621 0.026
Zn 0.889 0.778 0.001
Zn 0.056 0.945 0.001
Zn 0.056 0.778 0.001
Zn 0.889 0.944 0.001
Zn 0.889 0.611 0.001
Zn 0.222 0.944 0.001
Zn 0.722 0.278 0.001
Zn 0.722 0.111 0.001
Zn 0.556 0.111 0.001
Zn 0.724 0.780 0.001
Zn 0.724 0.611 0.001
Zn 0.223 0.780 0.001
Zn 0.223 0.109 0.001
Zn 0.053 0.611 0.001
Zn 0.053 0.109 0.001
O 0.778 0.222 0.880
O 0.611 0.222 0.880
O 0.611 0.055 0.880
O 0.945 0.889 0.880
O 0.945 0.722 0.880
O 0.111 0.889 0.880
O 0.778 0.389 0.879
O 0.778 0.056 0.879
O 0.445 0.056 0.879
O 0.777 0.722 0.879
O 0.111 0.722 0.879
O 0.111 0.056 0.879
O 0.945 0.389 0.879
O 0.945 0.222 0.879
O 0.611 0.889 0.879
O 0.611 0.389 0.879
O 0.444 0.889 0.879
O 0.444 0.222 0.879
O 0.944 0.555 0.878
O 0.944 0.055 0.878
O 0.778 0.890 0.878
O 0.778 0.555 0.878
O 0.278 0.890 0.878
O 0.278 0.055 0.878
O 0.445 0.388 0.875
O 0.445 0.724 0.875
O 0.109 0.388 0.875
O 0.612 0.724 0.875
O 0.612 0.555 0.875
O 0.278 0.724 0.875
O 0.278 0.221 0.875
O 0.110 0.555 0.875

O 0.110 0.221 0.875
O 0.889 0.778 0.380
O 0.056 0.945 0.380
O 0.056 0.778 0.380
O 0.722 0.278 0.380
O 0.722 0.111 0.380
O 0.556 0.111 0.380
O 0.889 0.944 0.379
O 0.889 0.611 0.379
O 0.222 0.944 0.379
O 0.889 0.278 0.379
O 0.555 0.944 0.379
O 0.555 0.278 0.379
O 0.722 0.778 0.379
O 0.722 0.611 0.379
O 0.223 0.778 0.379
O 0.223 0.111 0.379
O 0.055 0.611 0.379
O 0.055 0.111 0.379
O 0.888 0.445 0.378
O 0.888 0.110 0.378
O 0.723 0.945 0.378
O 0.723 0.445 0.378
O 0.389 0.945 0.378
O 0.389 0.110 0.378
O 0.557 0.612 0.375
O 0.221 0.612 0.375
O 0.221 0.276 0.375
O 0.557 0.779 0.375
O 0.557 0.445 0.375
O 0.389 0.779 0.375
O 0.389 0.276 0.375
O 0.055 0.445 0.375
O 0.055 0.276 0.375

Str 88 (WZ-ZnO-NP-2)
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.28 eV
E_{rel}: 0.23 eV/ZnO
$Pore_{max}$: 0.39 nm
V_{pore}: 10 %
D_{pore}: 1
cell parameters
9.935 9.877 5.348 90.00 90.00 120.19
fractional coordinates
Zn 0.780 0.226 1.000
Zn 0.774 0.555 0.999
Zn 0.114 0.555 0.999
Zn 0.443 0.231 0.998
Zn 0.121 0.231 0.998
Zn 0.578 0.420 0.526
Zn 0.176 0.420 0.526
Zn 0.890 0.446 0.503

Zn 0.220 0.107 0.500
Zn 0.886 0.779 0.499
Zn 0.226 0.779 0.499
Zn 0.879 0.103 0.498
Zn 0.557 0.103 0.498
Zn 0.422 0.913 0.026
Zn 0.824 0.913 0.026
Zn 0.110 0.887 0.003
O 0.890 0.448 0.877
O 0.221 0.109 0.877
O 0.890 0.777 0.874
O 0.220 0.777 0.874
O 0.889 0.114 0.873
O 0.558 0.114 0.873
O 0.563 0.442 0.872
O 0.213 0.442 0.872
O 0.110 0.886 0.377
O 0.779 0.225 0.377
O 0.780 0.556 0.374
O 0.110 0.556 0.374
O 0.111 0.219 0.373
O 0.442 0.219 0.373
O 0.437 0.891 0.372
O 0.787 0.891 0.372

Str 89 (WZ-ZnO-NP-3)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.32 eV
E_{rel}: 0.20 eV/ZnO
$Pore_{max}$: 0.36 nm
V_{pore}: 10 %
D_{pore}: 1
cell parameters
21.778 8.781 5.340 90.01 89.98 87.71
fractional coordinates
Zn 0.419 0.605 0.942
Zn 0.919 0.105 0.942
Zn 0.368 0.242 0.941
Zn 0.868 0.742 0.941
Zn 0.821 0.392 0.941
Zn 0.321 0.892 0.941
Zn 0.723 0.680 0.940
Zn 0.572 0.640 0.940
Zn 0.224 0.180 0.940
Zn 0.072 0.140 0.940
Zn 0.773 0.043 0.939
Zn 0.273 0.543 0.939
Zn 0.669 0.334 0.939
Zn 0.169 0.834 0.939
Zn 0.513 0.347 0.920
Zn 0.013 0.846 0.920
Zn 0.641 0.964 0.914
Zn 0.141 0.464 0.914

Zn 0.638 0.769 0.442
Zn 0.138 0.269 0.442
Zn 0.686 0.119 0.442
Zn 0.587 0.406 0.442
Zn 0.186 0.619 0.442
Zn 0.087 0.906 0.442
Zn 0.783 0.832 0.440
Zn 0.283 0.332 0.440
Zn 0.434 0.371 0.440
Zn 0.934 0.871 0.440
Zn 0.734 0.469 0.439
Zn 0.234 0.969 0.439
Zn 0.837 0.177 0.439
Zn 0.337 0.677 0.439
Zn 0.494 0.664 0.421
Zn 0.994 0.165 0.421
Zn 0.365 0.048 0.413
Zn 0.865 0.548 0.413
O 0.514 0.313 0.570
O 0.014 0.813 0.570
O 0.627 0.976 0.567
O 0.127 0.476 0.567
O 0.418 0.595 0.566
O 0.918 0.095 0.566
O 0.574 0.630 0.566
O 0.074 0.130 0.566
O 0.366 0.248 0.566
O 0.866 0.748 0.566
O 0.818 0.390 0.565
O 0.318 0.890 0.565
O 0.722 0.683 0.563
O 0.271 0.545 0.563
O 0.771 0.045 0.563
O 0.222 0.183 0.563
O 0.669 0.333 0.563
O 0.169 0.833 0.563
O 0.492 0.697 0.071
O 0.992 0.197 0.071
O 0.140 0.263 0.066
O 0.640 0.764 0.066
O 0.432 0.380 0.066
O 0.932 0.880 0.066
O 0.588 0.416 0.066
O 0.379 0.035 0.066
O 0.879 0.535 0.066
O 0.088 0.916 0.066
O 0.689 0.122 0.065
O 0.189 0.622 0.065
O 0.284 0.328 0.063
O 0.784 0.828 0.063
O 0.736 0.467 0.063
O 0.236 0.967 0.063

O 0.337 0.678 0.063
O 0.837 0.178 0.063

Str 90 (WZ-ZnO-NP-4)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.30 eV
E_{rel}: 0.12 eV/ZnO
$Pore_{max}$: 0.53 nm
V_{pore}: 11 %
D_{pore}: 1
cell parameters
16.415 16.415 5.322 90.00 90.00 120.00
fractional coordinates
Zn 0.669 0.933 0.999
Zn 0.669 0.737 0.999
Zn 0.263 0.933 0.999
Zn 0.263 0.331 0.999
Zn 0.067 0.737 0.999
Zn 0.067 0.331 0.999
Zn 0.467 0.734 0.999
Zn 0.266 0.734 0.999
Zn 0.266 0.533 0.999
Zn 0.466 0.933 0.998
Zn 0.466 0.534 0.998
Zn 0.067 0.534 0.998
Zn 0.709 0.854 0.527
Zn 0.146 0.854 0.527
Zn 0.146 0.291 0.527
Zn 0.531 0.867 0.501
Zn 0.531 0.665 0.501
Zn 0.335 0.867 0.501
Zn 0.335 0.469 0.501
Zn 0.133 0.469 0.501
Zn 0.133 0.665 0.501
Zn 0.333 0.667 0.501
Zn 0.933 0.669 0.499
Zn 0.933 0.263 0.499
Zn 0.737 0.669 0.499
Zn 0.737 0.067 0.499
Zn 0.331 0.263 0.499
Zn 0.331 0.067 0.499
Zn 0.734 0.467 0.499
Zn 0.734 0.266 0.499
Zn 0.533 0.266 0.499
Zn 0.933 0.466 0.498
Zn 0.534 0.466 0.498
Zn 0.534 0.067 0.498
Zn 0.854 0.709 0.027
Zn 0.854 0.146 0.027
Zn 0.291 0.146 0.027
Zn 0.867 0.531 0.001
Zn 0.867 0.335 0.001
Zn 0.665 0.531 0.001

Zn 0.665 0.133 0.001
Zn 0.469 0.335 0.001
Zn 0.469 0.133 0.001
Zn 0.667 0.333 0.001
O 0.333 0.667 0.879
O 0.733 0.467 0.878
O 0.733 0.267 0.878
O 0.533 0.267 0.878
O 0.534 0.867 0.878
O 0.534 0.666 0.878
O 0.334 0.867 0.878
O 0.334 0.466 0.878
O 0.133 0.666 0.878
O 0.133 0.466 0.878
O 0.731 0.865 0.876
O 0.135 0.865 0.876
O 0.135 0.269 0.876
O 0.934 0.666 0.876
O 0.934 0.268 0.876
O 0.732 0.666 0.876
O 0.732 0.066 0.876
O 0.334 0.268 0.876
O 0.334 0.066 0.876
O 0.934 0.467 0.876
O 0.533 0.467 0.876
O 0.533 0.066 0.876
O 0.667 0.333 0.379
O 0.467 0.733 0.378
O 0.267 0.733 0.378
O 0.267 0.533 0.378
O 0.867 0.534 0.378
O 0.867 0.334 0.378
O 0.666 0.534 0.378
O 0.666 0.133 0.378
O 0.466 0.334 0.378
O 0.466 0.133 0.378
O 0.865 0.731 0.376
O 0.865 0.135 0.376
O 0.269 0.135 0.376
O 0.666 0.732 0.376
O 0.666 0.934 0.376
O 0.268 0.934 0.376
O 0.268 0.334 0.376
O 0.066 0.732 0.376
O 0.066 0.334 0.376
O 0.467 0.934 0.376
O 0.467 0.533 0.376
O 0.066 0.533 0.376

Str 91 (WZ-ZnO-NP-5)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.26 eV
E_{rel}: 0.13 eV/ZnO

Pore$_{max}$: 0.78 nm
V$_{pore}$: 11 %
D$_{pore}$: 1
cell parameters
23.047 23.047 5.318 90.00 90.00 120.00
fractional coordinates
Zn 0.476 0.953 1.000
Zn 0.476 0.095 1.000
Zn 0.190 0.667 1.000
Zn 0.190 0.095 1.000
Zn 0.048 0.953 1.000
Zn 0.048 0.667 1.000
Zn 0.619 0.954 0.999
Zn 0.189 0.524 0.999
Zn 0.907 0.954 0.999
Zn 0.907 0.524 0.999
Zn 0.619 0.236 0.999
Zn 0.189 0.236 0.999
Zn 0.906 0.808 0.997
Zn 0.474 0.808 0.997
Zn 0.906 0.669 0.997
Zn 0.474 0.237 0.997
Zn 0.335 0.669 0.997
Zn 0.335 0.237 0.997
Zn 0.819 0.608 0.524
Zn 0.535 0.782 0.524
Zn 0.535 0.324 0.524
Zn 0.361 0.608 0.524
Zn 0.819 0.782 0.524
Zn 0.361 0.324 0.524
Zn 0.238 0.905 0.502
Zn 0.952 0.333 0.502
Zn 0.952 0.191 0.502
Zn 0.810 0.191 0.502
Zn 0.093 0.332 0.501
Zn 0.810 0.332 0.501
Zn 0.810 0.050 0.501
Zn 0.381 0.047 0.501
Zn 0.381 0.905 0.501
Zn 0.238 0.762 0.501
Zn 0.238 0.047 0.501
Zn 0.096 0.905 0.501
Zn 0.096 0.762 0.501
Zn 0.095 0.048 0.501
Zn 0.524 0.048 0.501
Zn 0.095 0.619 0.501
Zn 0.380 0.189 0.500
Zn 0.954 0.763 0.500
Zn 0.380 0.763 0.500
Zn 0.953 0.476 0.500
Zn 0.953 0.048 0.500
Zn 0.095 0.476 0.500

```
Zn 0.667 0.190 0.500
Zn 0.667 0.048 0.500
Zn 0.095 0.190 0.500
Zn 0.954 0.619 0.499
Zn 0.954 0.907 0.499
Zn 0.524 0.189 0.499
Zn 0.524 0.907 0.499
Zn 0.236 0.189 0.499
Zn 0.236 0.619 0.499
Zn 0.808 0.906 0.497
Zn 0.808 0.474 0.497
Zn 0.669 0.906 0.497
Zn 0.237 0.474 0.497
Zn 0.669 0.335 0.497
Zn 0.237 0.335 0.497
Zn 0.324 0.535 0.024
Zn 0.782 0.535 0.024
Zn 0.608 0.819 0.024
Zn 0.608 0.361 0.024
Zn 0.782 0.819 0.024
Zn 0.324 0.361 0.024
Zn 0.905 0.238 0.002
Zn 0.333 0.952 0.002
Zn 0.191 0.952 0.002
Zn 0.191 0.810 0.002
Zn 0.332 0.810 0.001
Zn 0.332 0.093 0.001
Zn 0.050 0.810 0.001
Zn 0.905 0.381 0.001
Zn 0.905 0.096 0.001
Zn 0.762 0.238 0.001
Zn 0.047 0.381 0.001
Zn 0.047 0.238 0.001
Zn 0.762 0.096 0.001
Zn 0.048 0.095 0.001
Zn 0.619 0.095 0.001
Zn 0.048 0.524 0.001
Zn 0.763 0.954 0.000
Zn 0.189 0.380 0.000
Zn 0.763 0.380 0.000
O 0.238 0.905 0.880
O 0.952 0.333 0.880
O 0.952 0.191 0.880
O 0.810 0.191 0.880
O 0.381 0.047 0.879
O 0.381 0.905 0.879
O 0.238 0.762 0.879
O 0.238 0.047 0.879
O 0.096 0.905 0.879
O 0.096 0.762 0.879
O 0.095 0.048 0.879
O 0.524 0.048 0.879
```

```
O 0.095 0.619 0.879
O 0.094 0.333 0.879
O 0.810 0.333 0.879
O 0.810 0.049 0.879
O 0.953 0.049 0.878
O 0.953 0.476 0.878
O 0.094 0.476 0.878
O 0.094 0.190 0.878
O 0.667 0.190 0.878
O 0.667 0.049 0.878
O 0.953 0.906 0.877
O 0.953 0.619 0.877
O 0.524 0.190 0.877
O 0.524 0.906 0.877
O 0.237 0.619 0.877
O 0.237 0.190 0.877
O 0.955 0.763 0.876
O 0.379 0.763 0.876
O 0.379 0.187 0.876
O 0.236 0.475 0.875
O 0.810 0.475 0.875
O 0.810 0.907 0.875
O 0.668 0.907 0.875
O 0.668 0.332 0.875
O 0.236 0.332 0.875
O 0.813 0.765 0.872
O 0.813 0.620 0.872
O 0.523 0.765 0.872
O 0.523 0.329 0.872
O 0.378 0.620 0.872
O 0.378 0.329 0.872
O 0.905 0.238 0.380
O 0.333 0.952 0.380
O 0.191 0.952 0.380
O 0.191 0.810 0.380
O 0.905 0.381 0.379
O 0.905 0.096 0.379
O 0.047 0.381 0.379
O 0.047 0.238 0.379
O 0.762 0.238 0.379
O 0.762 0.096 0.379
O 0.048 0.095 0.379
O 0.619 0.095 0.379
O 0.048 0.524 0.379
O 0.333 0.810 0.379
O 0.333 0.094 0.379
O 0.049 0.810 0.379
O 0.476 0.953 0.378
O 0.049 0.953 0.378
O 0.476 0.094 0.378
O 0.190 0.094 0.378
O 0.190 0.667 0.378
```

O 0.049 0.667 0.378
O 0.906 0.953 0.377
O 0.619 0.953 0.377
O 0.190 0.524 0.377
O 0.906 0.524 0.377
O 0.190 0.237 0.377
O 0.619 0.237 0.377
O 0.763 0.955 0.376
O 0.763 0.379 0.376
O 0.187 0.379 0.376
O 0.907 0.810 0.375
O 0.475 0.810 0.375
O 0.907 0.668 0.375
O 0.475 0.236 0.375
O 0.332 0.668 0.375
O 0.332 0.236 0.375
O 0.765 0.523 0.372
O 0.620 0.378 0.372
O 0.329 0.523 0.372
O 0.765 0.813 0.372
O 0.620 0.813 0.372
O 0.329 0.378 0.372

Str 92 (WZ-ZnO-NP-6)
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.28 eV
E_{rel}: 0.18 eV/ZnO
$Pore_{max}$: 0.56 nm
V_{pore}: 15 %
D_{pore}: 1
cell parameters
16.402 16.483 5.335 90.00 90.00 119.84
fractional coordinates
Zn 0.871 0.934 1.000
Zn 0.263 0.934 1.000
Zn 0.867 0.533 1.000
Zn 0.869 0.336 0.998
Zn 0.667 0.336 0.998
Zn 0.265 0.133 0.997
Zn 0.068 0.133 0.997
Zn 0.873 0.140 0.996
Zn 0.467 0.140 0.996
Zn 0.463 0.339 0.996
Zn 0.076 0.339 0.996
Zn 0.546 0.455 0.531
Zn 0.109 0.455 0.531
Zn 0.347 0.249 0.527
Zn 0.102 0.249 0.527
Zn 0.932 0.468 0.502
Zn 0.736 0.468 0.502
Zn 0.131 0.063 0.502
Zn 0.730 0.667 0.502
Zn 0.137 0.667 0.502

```
Zn 0.734 0.269 0.501
Zn 0.929 0.266 0.500
Zn 0.537 0.266 0.500
Zn 0.933 0.667 0.500
Zn 0.931 0.864 0.498
Zn 0.133 0.864 0.498
Zn 0.732 0.067 0.497
Zn 0.535 0.067 0.497
Zn 0.927 0.060 0.496
Zn 0.333 0.060 0.496
Zn 0.724 0.861 0.496
Zn 0.337 0.861 0.496
Zn 0.691 0.745 0.031
Zn 0.254 0.745 0.031
Zn 0.698 0.951 0.027
Zn 0.453 0.951 0.027
Zn 0.868 0.732 0.002
Zn 0.064 0.732 0.002
Zn 0.669 0.137 0.002
Zn 0.663 0.533 0.002
Zn 0.070 0.533 0.002
Zn 0.066 0.931 0.001
O 0.535 0.467 0.878
O 0.132 0.467 0.878
O 0.131 0.063 0.878
O 0.735 0.269 0.878
O 0.934 0.469 0.878
O 0.734 0.469 0.878
O 0.734 0.666 0.877
O 0.132 0.666 0.877
O 0.932 0.864 0.876
O 0.131 0.864 0.876
O 0.933 0.665 0.876
O 0.935 0.270 0.874
O 0.535 0.270 0.874
O 0.736 0.072 0.874
O 0.535 0.072 0.874
O 0.931 0.064 0.874
O 0.333 0.064 0.874
O 0.336 0.260 0.874
O 0.124 0.260 0.874
O 0.733 0.866 0.872
O 0.333 0.866 0.872
O 0.668 0.733 0.378
O 0.265 0.733 0.378
O 0.669 0.137 0.378
O 0.065 0.931 0.378
O 0.866 0.731 0.378
O 0.066 0.731 0.378
O 0.668 0.534 0.377
O 0.066 0.534 0.377
O 0.868 0.336 0.376
```

O 0.669 0.336 0.376
O 0.867 0.535 0.376
O 0.865 0.930 0.374
O 0.265 0.930 0.374
O 0.265 0.129 0.374
O 0.064 0.129 0.374
O 0.869 0.136 0.374
O 0.467 0.136 0.374
O 0.676 0.940 0.374
O 0.464 0.940 0.374
O 0.467 0.334 0.372
O 0.067 0.334 0.372

Str 93 (WZ-ZnO-NP-7)

$\Delta E_{gap}(PBE_{GW-fit})$: 0.44 eV

E_{rel}: 0.22 eV/ZnO

$Pore_{max}$: 0.54 nm

V_{pore}: 15 %

D_{pore}: 1

cell parameters

22.855 11.416 5.349 90.01 90.01 60.02

fractional coordinates

Zn 0.806 0.371 0.878
Zn 0.176 0.001 0.878
Zn 0.594 0.334 0.877
Zn 0.389 0.539 0.877
Zn 0.991 0.632 0.875
Zn 0.491 0.671 0.855
Zn 0.235 0.676 0.852
Zn 0.748 0.164 0.851
Zn 0.327 0.838 0.851
Zn 0.075 0.329 0.851
Zn 0.907 0.496 0.851
Zn 0.656 0.509 0.851
Zn 0.658 0.004 0.849
Zn 0.324 0.338 0.849
Zn 0.827 0.840 0.849
Zn 0.243 0.173 0.849
Zn 0.739 0.677 0.849
Zn 0.573 0.842 0.849
Zn 0.156 0.510 0.849
Zn 0.409 0.006 0.849
Zn 0.173 0.641 0.379
Zn 0.809 0.005 0.379
Zn 0.388 0.172 0.378
Zn 0.594 0.966 0.377
Zn 0.991 0.374 0.375
Zn 0.491 0.837 0.355
Zn 0.744 0.831 0.352
Zn 0.074 0.510 0.352
Zn 0.908 0.675 0.352
Zn 0.238 0.336 0.352

Zn 0.655 0.174 0.351
Zn 0.328 0.501 0.351
Zn 0.825 0.498 0.349
Zn 0.157 0.166 0.349
Zn 0.240 0.837 0.349
Zn 0.323 1.000 0.349
Zn 0.659 0.664 0.349
Zn 0.742 0.336 0.349
Zn 0.573 0.502 0.348
Zn 0.410 0.664 0.348
O 0.491 0.836 0.730
O 0.744 0.837 0.726
O 0.239 0.341 0.726
O 0.658 0.670 0.726
O 0.325 0.003 0.726
O 0.244 0.833 0.725
O 0.906 0.669 0.725
O 0.739 0.338 0.725
O 0.823 0.506 0.725
O 0.157 0.669 0.725
O 0.076 0.499 0.725
O 0.573 0.506 0.725
O 0.409 0.670 0.725
O 0.160 0.170 0.725
O 0.401 0.173 0.725
O 0.825 0.002 0.725
O 0.581 0.993 0.724
O 0.321 0.507 0.724
O 0.661 0.168 0.724
O 0.991 0.346 0.723
O 0.491 0.672 0.229
O 0.326 0.834 0.226
O 0.741 0.671 0.226
O 0.242 0.170 0.226
O 0.574 0.835 0.226
O 0.657 0.504 0.226
O 0.408 0.001 0.226
O 0.906 0.506 0.225
O 0.077 0.335 0.225
O 0.661 0.001 0.225
O 0.321 0.341 0.225
O 0.820 0.343 0.225
O 0.162 0.001 0.225
O 0.241 0.670 0.225
O 0.741 0.171 0.224
O 0.825 0.837 0.224
O 0.157 0.505 0.224
O 0.579 0.337 0.223
O 0.991 0.660 0.223
O 0.404 0.510 0.223

Str 94 (WZ-ZnO-NP-8)

$\Delta E_{gap}(PBE_{GW-fit})$: 0.38 eV
E_{rel}: 0.18 eV/ZnO
$Pore_{max}$: 0.78 nm
V_{pore}: 16 %
D_{pore}: 1
cell parameters
19.795 19.795 5.331 90.00 90.00 120.00
fractional coordinates
Zn 0.891 0.946 0.998
Zn 0.891 0.445 0.998
Zn 0.555 0.946 0.998
Zn 0.555 0.109 0.998
Zn 0.054 0.445 0.998
Zn 0.054 0.109 0.998
Zn 0.389 0.944 0.998
Zn 0.056 0.944 0.998
Zn 0.056 0.611 0.998
Zn 0.890 0.776 0.998
Zn 0.890 0.614 0.998
Zn 0.386 0.776 0.998
Zn 0.386 0.110 0.998
Zn 0.224 0.614 0.998
Zn 0.224 0.110 0.998
Zn 0.789 0.746 0.525
Zn 0.789 0.542 0.525
Zn 0.458 0.746 0.525
Zn 0.458 0.211 0.525
Zn 0.254 0.542 0.525
Zn 0.254 0.211 0.525
Zn 0.943 0.221 0.502
Zn 0.779 0.221 0.502
Zn 0.779 0.057 0.502
Zn 0.277 0.889 0.501
Zn 0.111 0.889 0.501
Zn 0.111 0.723 0.501
Zn 0.946 0.723 0.501
Zn 0.277 0.723 0.501
Zn 0.277 0.054 0.501
Zn 0.946 0.891 0.498
Zn 0.946 0.555 0.498
Zn 0.445 0.891 0.498
Zn 0.445 0.054 0.498
Zn 0.109 0.555 0.498
Zn 0.109 0.054 0.498
Zn 0.944 0.389 0.498
Zn 0.944 0.056 0.498
Zn 0.611 0.056 0.498
Zn 0.776 0.890 0.498
Zn 0.776 0.386 0.498
Zn 0.614 0.890 0.498
Zn 0.614 0.224 0.498
Zn 0.110 0.386 0.498

```
Zn 0.110 0.224 0.498
Zn 0.746 0.789 0.025
Zn 0.746 0.458 0.025
Zn 0.542 0.789 0.025
Zn 0.542 0.254 0.025
Zn 0.211 0.458 0.025
Zn 0.211 0.254 0.025
Zn 0.221 0.943 0.002
Zn 0.221 0.779 0.002
Zn 0.057 0.779 0.002
Zn 0.889 0.277 0.001
Zn 0.889 0.111 0.001
Zn 0.723 0.111 0.001
Zn 0.723 0.946 0.001
Zn 0.723 0.277 0.001
Zn 0.054 0.277 0.001
O 0.943 0.222 0.879
O 0.778 0.222 0.879
O 0.778 0.057 0.879
O 0.278 0.889 0.879
O 0.111 0.889 0.879
O 0.111 0.722 0.879
O 0.948 0.724 0.877
O 0.276 0.724 0.877
O 0.276 0.052 0.877
O 0.945 0.890 0.876
O 0.945 0.556 0.876
O 0.444 0.890 0.876
O 0.444 0.055 0.876
O 0.110 0.556 0.876
O 0.110 0.055 0.876
O 0.944 0.388 0.876
O 0.944 0.056 0.876
O 0.612 0.056 0.876
O 0.779 0.892 0.875
O 0.779 0.387 0.875
O 0.613 0.892 0.875
O 0.613 0.221 0.875
O 0.108 0.387 0.875
O 0.108 0.221 0.875
O 0.783 0.727 0.872
O 0.783 0.556 0.872
O 0.444 0.727 0.872
O 0.444 0.217 0.872
O 0.273 0.556 0.872
O 0.273 0.217 0.872
O 0.222 0.943 0.379
O 0.222 0.778 0.379
O 0.057 0.778 0.379
O 0.889 0.278 0.379
O 0.889 0.111 0.379
O 0.722 0.111 0.379
```

O 0.724 0.948 0.377
O 0.724 0.276 0.377
O 0.052 0.276 0.377
O 0.890 0.945 0.376
O 0.890 0.444 0.376
O 0.556 0.945 0.376
O 0.556 0.110 0.376
O 0.055 0.444 0.376
O 0.055 0.110 0.376
O 0.388 0.944 0.376
O 0.056 0.944 0.376
O 0.056 0.612 0.376
O 0.892 0.779 0.375
O 0.892 0.613 0.375
O 0.387 0.779 0.375
O 0.387 0.108 0.375
O 0.221 0.613 0.375
O 0.221 0.108 0.375
O 0.727 0.783 0.372
O 0.727 0.444 0.372
O 0.556 0.783 0.372
O 0.556 0.273 0.372
O 0.217 0.444 0.372
O 0.217 0.273 0.372

Str 95 (WZ-ZnO-NP-9)
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.44 eV
E_{rel}: 0.21 eV/ZnO
$Pore_{max}$: 0.52 nm
V_{pore}: 16 %
D_{pore}: 1
cell parameters
13.109 13.109 5.345 90.00 90.00 120.00
fractional coordinates
Zn 0.587 0.671 0.998
Zn 0.329 0.915 0.998
Zn 0.586 0.915 0.998
Zn 0.329 0.413 0.998
Zn 0.085 0.671 0.998
Zn 0.085 0.414 0.998
Zn 0.333 0.667 0.996
Zn 0.180 0.820 0.528
Zn 0.639 0.820 0.528
Zn 0.180 0.361 0.528
Zn 0.417 0.583 0.501
Zn 0.417 0.834 0.501
Zn 0.166 0.583 0.501
Zn 0.414 0.085 0.498
Zn 0.413 0.329 0.498
Zn 0.915 0.586 0.498
Zn 0.671 0.587 0.498
Zn 0.671 0.085 0.498

Zn 0.915 0.329 0.498
Zn 0.667 0.333 0.496
Zn 0.361 0.180 0.028
Zn 0.820 0.639 0.028
Zn 0.820 0.180 0.028
Zn 0.583 0.417 0.001
Zn 0.583 0.166 0.001
Zn 0.834 0.417 0.001
O 0.417 0.583 0.876
O 0.165 0.583 0.876
O 0.417 0.835 0.876
O 0.667 0.333 0.876
O 0.167 0.833 0.875
O 0.666 0.833 0.875
O 0.167 0.334 0.875
O 0.917 0.584 0.874
O 0.416 0.083 0.874
O 0.416 0.334 0.874
O 0.666 0.584 0.874
O 0.666 0.083 0.874
O 0.917 0.334 0.874
O 0.835 0.417 0.376
O 0.583 0.417 0.376
O 0.583 0.165 0.376
O 0.333 0.667 0.376
O 0.334 0.167 0.375
O 0.833 0.666 0.375
O 0.833 0.167 0.375
O 0.334 0.917 0.374
O 0.083 0.666 0.374
O 0.584 0.666 0.374
O 0.584 0.917 0.374
O 0.334 0.416 0.374
O 0.083 0.416 0.374

Str 96 (WZ-ZnO-NP-10)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.48 eV
E_{rel}: 0.25 eV/ZnO
$Pore_{max}$: 0.57 nm
V_{pore}: 20 %
D_{pore}: 1
cell parameters
13.172 26.428 5.356 90.00 90.01 119.92
fractional coordinates
Zn 0.181 0.690 0.882
Zn 0.928 0.690 0.881
Zn 0.923 0.411 0.879
Zn 0.633 0.915 0.879
Zn 0.176 0.914 0.878
Zn 0.183 0.193 0.869
Zn 0.187 0.535 0.866
Zn 0.165 0.799 0.853

Zn 0.907 0.292 0.852
Zn 0.912 0.802 0.852
Zn 0.415 0.798 0.852
Zn 0.664 0.674 0.851
Zn 0.412 0.923 0.851
Zn 0.659 0.296 0.851
Zn 0.415 0.674 0.851
Zn 0.159 0.298 0.851
Zn 0.668 0.800 0.851
Zn 0.908 0.167 0.849
Zn 0.164 0.419 0.849
Zn 0.664 0.046 0.849
Zn 0.407 0.047 0.849
Zn 0.422 0.304 0.848
Zn 0.658 0.169 0.847
Zn 0.410 0.170 0.847
Zn 0.426 0.547 0.847
Zn 0.563 0.321 0.382
Zn 0.566 0.600 0.380
Zn 0.810 0.095 0.379
Zn 0.359 0.096 0.378
Zn 0.815 0.824 0.378
Zn 0.304 0.316 0.375
Zn 0.302 0.476 0.367
Zn 0.578 0.717 0.354
Zn 0.582 0.212 0.353
Zn 0.831 0.712 0.353
Zn 0.827 0.339 0.353
Zn 0.575 0.086 0.352
Zn 0.826 0.213 0.352
Zn 0.074 0.338 0.351
Zn 0.322 0.208 0.351
Zn 0.071 0.209 0.350
Zn 0.584 0.842 0.350
Zn 0.328 0.715 0.349
Zn 0.324 0.593 0.349
Zn 0.580 0.962 0.349
Zn 0.323 0.962 0.349
Zn 0.080 0.840 0.347
Zn 0.075 0.710 0.347
Zn 0.064 0.464 0.347
Zn 0.329 0.839 0.345
O 0.581 0.717 0.728
O 0.579 0.212 0.727
O 0.580 0.337 0.727
O 0.072 0.337 0.727
O 0.825 0.211 0.727
O 0.575 0.086 0.726
O 0.826 0.335 0.726
O 0.831 0.717 0.726
O 0.584 0.594 0.725
O 0.824 0.088 0.725

O 0.333 0.090 0.725
O 0.332 0.715 0.725
O 0.330 0.839 0.725
O 0.580 0.840 0.724
O 0.078 0.838 0.724
O 0.828 0.839 0.724
O 0.328 0.964 0.724
O 0.079 0.714 0.724
O 0.577 0.963 0.724
O 0.073 0.213 0.724
O 0.317 0.330 0.723
O 0.333 0.214 0.721
O 0.334 0.592 0.720
O 0.072 0.462 0.719
O 0.317 0.471 0.717
O 0.908 0.295 0.228
O 0.168 0.677 0.227
O 0.665 0.676 0.227
O 0.415 0.799 0.226
O 0.661 0.294 0.226
O 0.162 0.797 0.226
O 0.414 0.674 0.226
O 0.659 0.169 0.226
O 0.412 0.922 0.226
O 0.915 0.675 0.226
O 0.660 0.922 0.225
O 0.162 0.920 0.225
O 0.663 0.799 0.225
O 0.913 0.797 0.225
O 0.154 0.295 0.225
O 0.906 0.418 0.225
O 0.907 0.170 0.224
O 0.409 0.045 0.224
O 0.414 0.172 0.224
O 0.659 0.045 0.224
O 0.413 0.297 0.221
O 0.155 0.419 0.221
O 0.417 0.550 0.219
O 0.167 0.178 0.217
O 0.172 0.540 0.215

Str 97 (WZ-ZnO-NP-11)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.37 eV
E_{rel}: 0.16 eV/ZnO
$Pore_{max}$: 1.12 nm
V_{pore}: 22 %
D_{pore}: 1
cell parameters
26.269 26.317 5.335 90.01 90.00 119.94
fractional coordinates
Zn 0.088 0.313 0.882
Zn 0.215 0.313 0.882

Zn 0.087 0.788 0.881
Zn 0.691 0.788 0.881
Zn 0.464 0.938 0.880
Zn 0.464 0.663 0.879
Zn 0.189 0.663 0.879
Zn 0.215 0.914 0.877
Zn 0.688 0.914 0.877
Zn 0.078 0.670 0.853
Zn 0.581 0.670 0.852
Zn 0.955 0.673 0.852
Zn 0.707 0.673 0.852
Zn 0.330 0.296 0.852
Zn 0.955 0.296 0.852
Zn 0.208 0.795 0.852
Zn 0.576 0.795 0.852
Zn 0.079 0.545 0.851
Zn 0.455 0.545 0.851
Zn 0.333 0.423 0.851
Zn 0.207 0.425 0.851
Zn 0.080 0.423 0.851
Zn 0.329 0.048 0.851
Zn 0.333 0.921 0.851
Zn 0.708 0.048 0.851
Zn 0.578 0.921 0.851
Zn 0.583 0.049 0.850
Zn 0.456 0.049 0.850
Zn 0.330 0.548 0.850
Zn 0.207 0.548 0.850
Zn 0.706 0.422 0.850
Zn 0.581 0.297 0.850
Zn 0.706 0.297 0.850
Zn 0.581 0.422 0.850
Zn 0.581 0.172 0.849
Zn 0.830 0.422 0.849
Zn 0.456 0.422 0.849
Zn 0.955 0.422 0.849
Zn 0.955 0.546 0.849
Zn 0.581 0.546 0.849
Zn 0.326 0.170 0.849
Zn 0.833 0.677 0.849
Zn 0.834 0.170 0.848
Zn 0.831 0.548 0.848
Zn 0.706 0.548 0.848
Zn 0.831 0.296 0.848
Zn 0.455 0.172 0.848
Zn 0.455 0.296 0.848
Zn 0.707 0.172 0.848
Zn 0.305 0.097 0.383
Zn 0.781 0.097 0.383
Zn 0.305 0.223 0.383
Zn 0.907 0.223 0.383
Zn 0.907 0.697 0.382

Zn 0.780 0.697 0.382
Zn 0.280 0.571 0.377
Zn 0.560 0.848 0.372
Zn 0.278 0.848 0.372
Zn 0.788 0.586 0.352
Zn 0.288 0.966 0.352
Zn 0.668 0.966 0.352
Zn 0.288 0.337 0.352
Zn 0.039 0.337 0.352
Zn 0.417 0.215 0.352
Zn 0.788 0.215 0.352
Zn 0.416 0.341 0.352
Zn 0.914 0.586 0.352
Zn 0.914 0.341 0.352
Zn 0.662 0.586 0.352
Zn 0.416 0.089 0.351
Zn 0.662 0.089 0.351
Zn 0.039 0.715 0.351
Zn 0.665 0.715 0.351
Zn 0.789 0.463 0.351
Zn 0.664 0.463 0.351
Zn 0.664 0.339 0.350
Zn 0.789 0.339 0.350
Zn 0.540 0.339 0.350
Zn 0.539 0.214 0.350
Zn 0.664 0.214 0.350
Zn 0.539 0.463 0.350
Zn 0.913 0.464 0.350
Zn 0.414 0.590 0.350
Zn 0.165 0.590 0.349
Zn 0.537 0.962 0.349
Zn 0.414 0.962 0.349
Zn 0.539 0.088 0.349
Zn 0.289 0.460 0.349
Zn 0.161 0.460 0.349
Zn 0.158 0.841 0.348
Zn 0.162 0.334 0.348
Zn 0.673 0.841 0.348
Zn 0.415 0.464 0.348
Zn 0.039 0.464 0.348
Zn 0.040 0.589 0.348
Zn 0.538 0.589 0.348
Zn 0.538 0.713 0.348
Zn 0.165 0.713 0.348
O 0.291 0.216 0.729
O 0.291 0.090 0.729
O 0.788 0.090 0.729
O 0.914 0.216 0.729
O 0.914 0.712 0.729
O 0.787 0.712 0.729
O 0.664 0.339 0.728
O 0.789 0.464 0.728

O 0.789 0.339 0.728
O 0.664 0.464 0.728
O 0.664 0.214 0.728
O 0.539 0.339 0.728
O 0.539 0.214 0.728
O 0.914 0.588 0.727
O 0.789 0.589 0.727
O 0.663 0.588 0.727
O 0.914 0.339 0.727
O 0.414 0.339 0.727
O 0.290 0.340 0.727
O 0.039 0.340 0.727
O 0.414 0.214 0.727
O 0.790 0.214 0.727
O 0.539 0.089 0.727
O 0.163 0.463 0.727
O 0.290 0.463 0.727
O 0.414 0.089 0.727
O 0.291 0.965 0.726
O 0.665 0.089 0.726
O 0.539 0.463 0.726
O 0.664 0.965 0.726
O 0.913 0.463 0.726
O 0.038 0.712 0.726
O 0.664 0.712 0.726
O 0.039 0.588 0.726
O 0.538 0.588 0.726
O 0.414 0.587 0.726
O 0.163 0.587 0.726
O 0.540 0.713 0.725
O 0.162 0.713 0.725
O 0.287 0.585 0.725
O 0.415 0.463 0.725
O 0.164 0.339 0.725
O 0.038 0.463 0.725
O 0.540 0.965 0.725
O 0.415 0.965 0.725
O 0.162 0.838 0.723
O 0.665 0.838 0.723
O 0.286 0.842 0.720
O 0.545 0.842 0.720
O 0.081 0.299 0.229
O 0.208 0.299 0.229
O 0.706 0.422 0.228
O 0.706 0.297 0.228
O 0.581 0.297 0.228
O 0.079 0.671 0.228
O 0.581 0.671 0.227
O 0.581 0.172 0.227
O 0.206 0.422 0.227
O 0.457 0.671 0.227
O 0.203 0.671 0.227

O 0.581 0.422 0.227
O 0.956 0.299 0.227
O 0.078 0.795 0.227
O 0.332 0.299 0.227
O 0.830 0.422 0.227
O 0.706 0.795 0.227
O 0.831 0.547 0.227
O 0.705 0.547 0.227
O 0.079 0.421 0.227
O 0.704 0.670 0.227
O 0.332 0.421 0.227
O 0.955 0.670 0.227
O 0.081 0.546 0.227
O 0.455 0.546 0.227
O 0.456 0.924 0.226
O 0.831 0.298 0.226
O 0.456 0.172 0.226
O 0.705 0.172 0.226
O 0.456 0.047 0.226
O 0.332 0.048 0.226
O 0.706 0.048 0.226
O 0.456 0.298 0.226
O 0.580 0.047 0.226
O 0.956 0.546 0.226
O 0.331 0.545 0.226
O 0.204 0.545 0.226
O 0.580 0.546 0.226
O 0.457 0.423 0.226
O 0.955 0.423 0.225
O 0.208 0.921 0.225
O 0.702 0.920 0.225
O 0.830 0.671 0.225
O 0.331 0.924 0.225
O 0.582 0.924 0.225
O 0.331 0.173 0.225
O 0.831 0.173 0.225
O 0.583 0.796 0.224
O 0.202 0.796 0.224

Str 98 (WZ-ZnO-NP-12)
$\Delta E_{gap}(PBE_{GW\text{-}fit})$: 0.33 eV
E_{rel}: 0.15 eV/ZnO
$Pore_{max}$: 1.12 nm
V_{pore}: 23 %
D_{pore}: 1
cell parameters
22.980 22.980 5.327 90.00 90.00 120.00
fractional coordinates
Zn 0.905 0.238 0.998
Zn 0.620 0.096 0.997
Zn 0.047 0.523 0.997
Zn 0.047 0.096 0.997

Zn 0.904 0.381 0.997
Zn 0.904 0.094 0.997
Zn 0.762 0.239 0.997
Zn 0.762 0.094 0.997
Zn 0.049 0.381 0.997
Zn 0.049 0.239 0.997
Zn 0.759 0.946 0.996
Zn 0.759 0.384 0.996
Zn 0.197 0.384 0.996
Zn 0.819 0.922 0.530
Zn 0.819 0.468 0.530
Zn 0.675 0.922 0.530
Zn 0.675 0.324 0.530
Zn 0.221 0.468 0.530
Zn 0.221 0.324 0.530
Zn 0.811 0.332 0.501
Zn 0.811 0.050 0.501
Zn 0.093 0.332 0.501
Zn 0.954 0.476 0.501
Zn 0.954 0.049 0.501
Zn 0.666 0.189 0.501
Zn 0.666 0.049 0.501
Zn 0.094 0.476 0.501
Zn 0.094 0.189 0.501
Zn 0.951 0.903 0.500
Zn 0.951 0.620 0.500
Zn 0.523 0.903 0.500
Zn 0.523 0.192 0.500
Zn 0.240 0.620 0.500
Zn 0.240 0.192 0.500
Zn 0.952 0.333 0.500
Zn 0.952 0.191 0.500
Zn 0.810 0.191 0.500
Zn 0.238 0.905 0.498
Zn 0.523 0.047 0.497
Zn 0.096 0.620 0.497
Zn 0.096 0.047 0.497
Zn 0.381 0.904 0.497
Zn 0.381 0.049 0.497
Zn 0.239 0.762 0.497
Zn 0.239 0.049 0.497
Zn 0.094 0.904 0.497
Zn 0.094 0.762 0.497
Zn 0.946 0.759 0.496
Zn 0.384 0.759 0.496
Zn 0.384 0.197 0.496
Zn 0.922 0.819 0.030
Zn 0.922 0.675 0.030
Zn 0.468 0.819 0.030
Zn 0.468 0.221 0.030
Zn 0.324 0.675 0.030
Zn 0.324 0.221 0.030

Zn 0.332 0.811 0.001
Zn 0.332 0.093 0.001
Zn 0.050 0.811 0.001
Zn 0.476 0.954 0.001
Zn 0.476 0.094 0.001
Zn 0.189 0.666 0.001
Zn 0.189 0.094 0.001
Zn 0.049 0.954 0.001
Zn 0.049 0.666 0.001
Zn 0.903 0.951 0.000
Zn 0.903 0.523 0.000
Zn 0.620 0.951 0.000
Zn 0.620 0.240 0.000
Zn 0.192 0.523 0.000
Zn 0.192 0.240 0.000
Zn 0.333 0.952 0.000
Zn 0.191 0.952 0.000
Zn 0.191 0.810 0.000
O 0.953 0.334 0.878
O 0.953 0.190 0.878
O 0.809 0.190 0.878
O 0.811 0.906 0.878
O 0.811 0.476 0.878
O 0.666 0.906 0.878
O 0.666 0.332 0.878
O 0.237 0.476 0.878
O 0.237 0.332 0.878
O 0.238 0.905 0.877
O 0.953 0.476 0.876
O 0.953 0.048 0.876
O 0.666 0.190 0.876
O 0.666 0.048 0.876
O 0.095 0.476 0.876
O 0.095 0.190 0.876
O 0.809 0.334 0.876
O 0.809 0.046 0.876
O 0.096 0.334 0.876
O 0.381 0.905 0.876
O 0.381 0.048 0.876
O 0.238 0.762 0.876
O 0.238 0.048 0.876
O 0.095 0.905 0.876
O 0.095 0.762 0.876
O 0.953 0.906 0.876
O 0.953 0.619 0.876
O 0.524 0.906 0.876
O 0.524 0.189 0.876
O 0.237 0.619 0.876
O 0.237 0.189 0.876
O 0.525 0.048 0.874
O 0.095 0.618 0.874
O 0.095 0.048 0.874

O 0.952 0.762 0.874
O 0.381 0.762 0.874
O 0.381 0.191 0.874
O 0.334 0.953 0.378
O 0.190 0.953 0.378
O 0.190 0.809 0.378
O 0.906 0.811 0.378
O 0.906 0.666 0.378
O 0.476 0.811 0.378
O 0.476 0.237 0.378
O 0.332 0.666 0.378
O 0.332 0.237 0.378
O 0.905 0.238 0.377
O 0.476 0.953 0.377
O 0.476 0.095 0.377
O 0.190 0.666 0.377
O 0.190 0.095 0.377
O 0.048 0.953 0.377
O 0.048 0.666 0.377
O 0.334 0.809 0.376
O 0.334 0.096 0.376
O 0.046 0.809 0.376
O 0.905 0.381 0.376
O 0.905 0.095 0.376
O 0.762 0.238 0.376
O 0.762 0.095 0.376
O 0.048 0.381 0.376
O 0.048 0.238 0.376
O 0.906 0.953 0.376
O 0.906 0.524 0.376
O 0.619 0.953 0.376
O 0.619 0.237 0.376
O 0.189 0.524 0.376
O 0.189 0.237 0.376
O 0.618 0.095 0.374
O 0.048 0.525 0.374
O 0.048 0.095 0.374
O 0.762 0.952 0.374
O 0.762 0.381 0.374
O 0.191 0.381 0.374

Str 99 (WZ-ZnO-NP-13)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.36 eV
E_{rel}: 0.21 eV/ZnO
$Pore_{max}$: 0.94 nm
V_{pore}: 24 %
D_{pore}: 1
cell parameters
19.810 19.810 5.342 90.00 90.00 120.51
fractional coordinates
Zn 0.386 0.109 1.000
Zn 0.058 0.781 1.000

Zn 0.056 0.111 0.999
Zn 0.386 0.944 0.998
Zn 0.223 0.780 0.998
Zn 0.718 0.935 0.998
Zn 0.232 0.448 0.998
Zn 0.058 0.277 0.997
Zn 0.889 0.109 0.997
Zn 0.552 0.104 0.997
Zn 0.063 0.615 0.997
Zn 0.552 0.939 0.996
Zn 0.228 0.614 0.996
Zn 0.723 0.105 0.995
Zn 0.062 0.444 0.995
Zn 0.788 0.909 0.532
Zn 0.258 0.379 0.532
Zn 0.621 0.912 0.531
Zn 0.255 0.545 0.531
Zn 0.456 0.917 0.527
Zn 0.250 0.711 0.527
Zn 0.947 0.056 0.502
Zn 0.111 0.220 0.502
Zn 0.941 0.886 0.502
Zn 0.281 0.225 0.502
Zn 0.275 0.891 0.502
Zn 0.946 0.221 0.500
Zn 0.781 0.058 0.500
Zn 0.109 0.386 0.500
Zn 0.111 0.056 0.499
Zn 0.944 0.386 0.498
Zn 0.780 0.223 0.498
Zn 0.935 0.718 0.498
Zn 0.448 0.232 0.498
Zn 0.277 0.058 0.497
Zn 0.109 0.889 0.497
Zn 0.104 0.552 0.497
Zn 0.615 0.063 0.497
Zn 0.939 0.552 0.496
Zn 0.614 0.228 0.496
Zn 0.105 0.723 0.495
Zn 0.444 0.062 0.495
Zn 0.909 0.788 0.032
Zn 0.379 0.258 0.032
Zn 0.912 0.621 0.032
Zn 0.545 0.255 0.032
Zn 0.917 0.456 0.027
Zn 0.711 0.250 0.027
Zn 0.220 0.111 0.002
Zn 0.056 0.947 0.002
Zn 0.886 0.941 0.002
Zn 0.225 0.281 0.002
Zn 0.891 0.275 0.002
Zn 0.221 0.946 0.000

```
O 0.779 0.889 0.878
O 0.277 0.388 0.878
O 0.945 0.054 0.877
O 0.113 0.221 0.877
O 0.612 0.893 0.877
O 0.274 0.555 0.877
O 0.275 0.891 0.877
O 0.944 0.889 0.877
O 0.277 0.222 0.877
O 0.946 0.221 0.877
O 0.110 0.056 0.875
O 0.276 0.057 0.875
O 0.110 0.891 0.875
O 0.779 0.052 0.874
O 0.114 0.388 0.874
O 0.947 0.386 0.874
O 0.780 0.219 0.874
O 0.943 0.722 0.874
O 0.445 0.224 0.874
O 0.447 0.899 0.873
O 0.268 0.720 0.873
O 0.442 0.058 0.873
O 0.109 0.724 0.873
O 0.110 0.554 0.872
O 0.613 0.057 0.872
O 0.947 0.556 0.872
O 0.611 0.220 0.872
O 0.889 0.779 0.378
O 0.388 0.277 0.378
O 0.221 0.112 0.377
O 0.054 0.945 0.377
O 0.893 0.612 0.377
O 0.555 0.274 0.377
O 0.891 0.275 0.377
O 0.889 0.944 0.377
O 0.222 0.277 0.377
O 0.221 0.946 0.377
O 0.056 0.110 0.375
O 0.057 0.276 0.375
O 0.891 0.110 0.375
O 0.388 0.114 0.374
O 0.052 0.779 0.374
O 0.386 0.947 0.374
O 0.219 0.780 0.374
O 0.722 0.943 0.374
O 0.224 0.445 0.374
O 0.899 0.447 0.373
O 0.720 0.268 0.373
O 0.058 0.442 0.373
O 0.724 0.109 0.373
O 0.554 0.110 0.372
O 0.057 0.613 0.372
```

O 0.556 0.947 0.372
O 0.220 0.611 0.372

Str 100 (WZ-ZnO-NP-14)
$\Delta E_{gap}(PBE_{GW\text{-fit}})$: 0.58 eV
E_{rel}: 0.29 eV/ZnO
$Pore_{max}$: 0.57 nm
V_{pore}: 24 %
D_{pore}: 1
cell parameters
13.242 13.242 5.374 90.00 90.00 119.71
fractional coordinates
Zn 0.827 0.409 1.000
Zn 0.591 0.173 1.000
Zn 0.336 0.664 0.999
Zn 0.598 0.919 0.997
Zn 0.081 0.402 0.997
Zn 0.184 0.364 0.530
Zn 0.636 0.816 0.530
Zn 0.939 0.382 0.518
Zn 0.618 0.061 0.518
Zn 0.419 0.581 0.505
Zn 0.669 0.586 0.502
Zn 0.414 0.331 0.502
Zn 0.409 0.827 0.500
Zn 0.173 0.591 0.500
Zn 0.664 0.336 0.499
Zn 0.402 0.081 0.497
Zn 0.919 0.598 0.497
Zn 0.364 0.184 0.030
Zn 0.816 0.636 0.030
Zn 0.382 0.939 0.018
Zn 0.061 0.618 0.018
Zn 0.581 0.419 0.005
Zn 0.586 0.669 0.002
Zn 0.331 0.414 0.002
O 0.419 0.581 0.878
O 0.665 0.582 0.876
O 0.418 0.335 0.876
O 0.664 0.336 0.875
O 0.172 0.336 0.875
O 0.664 0.828 0.875
O 0.418 0.828 0.870
O 0.172 0.582 0.870
O 0.415 0.086 0.869
O 0.914 0.585 0.869
O 0.928 0.357 0.866
O 0.643 0.072 0.866
O 0.581 0.419 0.378
O 0.335 0.418 0.376
O 0.582 0.665 0.376
O 0.336 0.664 0.375

O 0.828 0.664 0.375
O 0.336 0.172 0.375
O 0.828 0.418 0.370
O 0.582 0.172 0.370
O 0.086 0.415 0.369
O 0.585 0.914 0.369
O 0.357 0.928 0.366
O 0.072 0.643 0.366

Str 101 (WZ-ZnO-NP-15)
ΔE_{gap}(PBE$_{GW-fit}$): 0.72 eV
E_{rel}: 0.28 eV/ZnO
Pore$_{max}$: 0.56 nm
V_{pore}: 25 %
D_{pore}: 1
cell parameters
11.516 11.520 5.365 89.99 90.03 119.99
fractional coordinates
Zn 0.312 0.000 0.565
Zn 0.937 0.376 0.564
Zn 0.561 0.625 0.564
Zn 0.430 0.326 0.540
Zn 0.611 0.168 0.540
Zn 0.104 0.674 0.540
Zn 0.263 0.494 0.540
Zn 0.769 0.506 0.540
Zn 0.443 0.833 0.540
Zn 0.561 1.000 0.064
Zn 0.312 0.375 0.064
Zn 0.936 0.625 0.064
Zn 0.430 0.167 0.041
Zn 0.263 0.833 0.040
Zn 0.610 0.506 0.040
Zn 0.104 0.494 0.040
Zn 0.769 0.326 0.040
Zn 0.443 0.674 0.040
O 0.440 0.334 0.914
O 0.106 0.666 0.914
O 0.602 0.169 0.914
O 0.270 0.504 0.913
O 0.767 0.496 0.913
O 0.433 0.831 0.913
O 0.284 0.000 0.912
O 0.936 0.348 0.912
O 0.588 0.652 0.912
O 0.440 0.169 0.414
O 0.271 0.831 0.414
O 0.602 0.496 0.413
O 0.106 0.504 0.413
O 0.767 0.334 0.413
O 0.433 0.666 0.413
O 0.589 0.000 0.412

O 0.284 0.348 0.412
O 0.936 0.652 0.411

Str 102 (WZ-ZnO-NP-16)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.39 eV
E_{rel}: 0.20 eV/ZnO
$Pore_{max}$: 1.12 nm
V_{pore}: 25 %
D_{pore}: 1
cell parameters
23.039 23.062 5.342 89.99 90.00 119.97
fractional coordinates
Zn 0.100 0.357 0.882
Zn 0.244 0.357 0.882
Zn 0.098 0.759 0.881
Zn 0.648 0.758 0.881
Zn 0.390 0.614 0.877
Zn 0.212 0.614 0.877
Zn 0.246 0.901 0.874
Zn 0.643 0.901 0.874
Zn 0.236 0.485 0.855
Zn 0.087 0.623 0.853
Zn 0.523 0.622 0.853
Zn 0.089 0.481 0.852
Zn 0.380 0.481 0.852
Zn 0.948 0.337 0.852
Zn 0.947 0.626 0.852
Zn 0.666 0.626 0.851
Zn 0.377 0.337 0.851
Zn 0.235 0.766 0.851
Zn 0.518 0.766 0.851
Zn 0.666 0.055 0.851
Zn 0.377 0.055 0.851
Zn 0.521 0.055 0.850
Zn 0.380 0.910 0.849
Zn 0.518 0.910 0.849
Zn 0.948 0.482 0.849
Zn 0.521 0.482 0.849
Zn 0.809 0.195 0.848
Zn 0.664 0.340 0.848
Zn 0.373 0.195 0.848
Zn 0.809 0.630 0.848
Zn 0.664 0.197 0.847
Zn 0.807 0.339 0.847
Zn 0.521 0.197 0.847
Zn 0.520 0.339 0.847
Zn 0.664 0.483 0.847
Zn 0.806 0.483 0.847
Zn 0.750 0.112 0.383
Zn 0.350 0.112 0.383
Zn 0.893 0.254 0.382
Zn 0.349 0.254 0.382

Zn 0.749 0.654 0.382
Zn 0.893 0.654 0.381
Zn 0.315 0.828 0.369
Zn 0.501 0.828 0.369
Zn 0.476 0.102 0.352
Zn 0.614 0.102 0.352
Zn 0.757 0.247 0.352
Zn 0.477 0.247 0.352
Zn 0.473 0.958 0.352
Zn 0.329 0.962 0.352
Zn 0.621 0.962 0.352
Zn 0.757 0.526 0.352
Zn 0.902 0.389 0.351
Zn 0.902 0.528 0.351
Zn 0.475 0.389 0.351
Zn 0.614 0.528 0.351
Zn 0.043 0.674 0.351
Zn 0.619 0.674 0.351
Zn 0.616 0.245 0.350
Zn 0.328 0.385 0.350
Zn 0.045 0.385 0.350
Zn 0.616 0.387 0.350
Zn 0.759 0.387 0.350
Zn 0.184 0.381 0.348
Zn 0.179 0.819 0.348
Zn 0.628 0.819 0.348
Zn 0.045 0.530 0.347
Zn 0.186 0.672 0.347
Zn 0.474 0.672 0.347
Zn 0.472 0.530 0.347
Zn 0.188 0.530 0.345
Zn 0.330 0.530 0.345
O 0.758 0.103 0.729
O 0.333 0.103 0.729
O 0.901 0.246 0.728
O 0.333 0.246 0.728
O 0.616 0.102 0.727
O 0.474 0.102 0.727
O 0.757 0.670 0.727
O 0.901 0.670 0.727
O 0.616 0.245 0.727
O 0.474 0.960 0.727
O 0.759 0.387 0.727
O 0.616 0.387 0.727
O 0.902 0.387 0.727
O 0.759 0.245 0.727
O 0.473 0.245 0.727
O 0.473 0.387 0.727
O 0.902 0.529 0.727
O 0.616 0.529 0.727
O 0.759 0.530 0.726
O 0.042 0.672 0.726

O 0.331 0.386 0.726
O 0.617 0.671 0.726
O 0.044 0.386 0.726
O 0.617 0.961 0.726
O 0.332 0.961 0.726
O 0.044 0.529 0.725
O 0.187 0.387 0.725
O 0.473 0.529 0.725
O 0.186 0.528 0.724
O 0.183 0.672 0.724
O 0.476 0.672 0.724
O 0.330 0.528 0.724
O 0.184 0.816 0.722
O 0.620 0.815 0.721
O 0.324 0.821 0.718
O 0.484 0.821 0.718
O 0.236 0.341 0.228
O 0.092 0.341 0.228
O 0.234 0.481 0.228
O 0.089 0.624 0.227
O 0.523 0.624 0.227
O 0.088 0.766 0.227
O 0.521 0.053 0.227
O 0.665 0.766 0.227
O 0.091 0.481 0.227
O 0.664 0.340 0.227
O 0.378 0.481 0.227
O 0.663 0.197 0.226
O 0.663 0.056 0.226
O 0.521 0.197 0.226
O 0.380 0.056 0.226
O 0.949 0.341 0.226
O 0.807 0.340 0.226
O 0.379 0.341 0.226
O 0.521 0.340 0.226
O 0.663 0.482 0.226
O 0.948 0.623 0.226
O 0.663 0.623 0.226
O 0.807 0.482 0.226
O 0.950 0.482 0.225
O 0.521 0.482 0.225
O 0.382 0.622 0.225
O 0.227 0.622 0.225
O 0.807 0.198 0.224
O 0.379 0.198 0.224
O 0.522 0.913 0.224
O 0.379 0.913 0.224
O 0.806 0.624 0.224
O 0.239 0.909 0.223
O 0.658 0.909 0.223
O 0.229 0.767 0.223
O 0.525 0.767 0.222

Str 103 (WZ-ZnO-NP-17)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.53 eV
E_{rel}: 0.27 eV/ZnO
$Pore_{max}$: 0.83 nm
V_{pore}: 29 %
D_{pore}: 1
cell parameters
16.447 16.447 5.358 90.00 90.00 120.78
fractional coordinates
Zn 0.862 0.929 0.999
Zn 0.070 0.138 0.999
Zn 0.867 0.331 0.996
Zn 0.669 0.133 0.996
Zn 0.661 0.922 0.995
Zn 0.078 0.339 0.995
Zn 0.868 0.132 0.992
Zn 0.743 0.887 0.530
Zn 0.113 0.257 0.530
Zn 0.542 0.890 0.528
Zn 0.110 0.458 0.528
Zn 0.747 0.253 0.527
Zn 0.935 0.065 0.501
Zn 0.935 0.265 0.501
Zn 0.735 0.065 0.501
Zn 0.928 0.467 0.500
Zn 0.533 0.072 0.500
Zn 0.929 0.862 0.499
Zn 0.138 0.070 0.499
Zn 0.331 0.867 0.496
Zn 0.133 0.669 0.496
Zn 0.922 0.661 0.495
Zn 0.339 0.078 0.495
Zn 0.132 0.868 0.492
Zn 0.887 0.743 0.030
Zn 0.257 0.113 0.030
Zn 0.890 0.542 0.028
Zn 0.458 0.110 0.028
Zn 0.253 0.747 0.027
Zn 0.065 0.935 0.001
Zn 0.265 0.935 0.001
Zn 0.065 0.735 0.001
Zn 0.467 0.928 0.000
Zn 0.072 0.533 0.000
O 0.733 0.865 0.876
O 0.135 0.267 0.876
O 0.935 0.065 0.875
O 0.938 0.267 0.874
O 0.733 0.062 0.874
O 0.737 0.263 0.874
O 0.931 0.866 0.873
O 0.134 0.069 0.873

O 0.531 0.866 0.873
O 0.134 0.469 0.873
O 0.935 0.466 0.873
O 0.534 0.065 0.873
O 0.132 0.868 0.872
O 0.333 0.871 0.872
O 0.129 0.667 0.872
O 0.928 0.664 0.871
O 0.336 0.072 0.871
O 0.865 0.733 0.376
O 0.267 0.135 0.376
O 0.065 0.935 0.375
O 0.267 0.938 0.374
O 0.062 0.733 0.374
O 0.263 0.737 0.374
O 0.866 0.931 0.373
O 0.069 0.134 0.373
O 0.866 0.531 0.373
O 0.469 0.134 0.373
O 0.466 0.935 0.373
O 0.065 0.534 0.373
O 0.868 0.132 0.372
O 0.871 0.333 0.372
O 0.667 0.129 0.372
O 0.664 0.928 0.371
O 0.072 0.336 0.371

Str 104 (WZ-ZnO-NP-18)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.46 eV
E_{rel}: 0.23 eV/ZnO
$Pore_{max}$: 1.12 nm
V_{pore}: 31 %
D_{pore}: 1
cell parameters
19.707 19.707 5.351 90.00 90.00 120.00
fractional coordinates
Zn 0.557 0.943 0.999
Zn 0.557 0.614 0.999
Zn 0.386 0.943 0.999
Zn 0.386 0.443 0.999
Zn 0.057 0.614 0.999
Zn 0.057 0.443 0.999
Zn 0.721 0.442 0.999
Zn 0.721 0.279 0.999
Zn 0.558 0.279 0.999
Zn 0.562 0.781 0.996
Zn 0.219 0.781 0.996
Zn 0.219 0.438 0.996
Zn 0.389 0.778 0.991
Zn 0.389 0.611 0.991
Zn 0.222 0.611 0.991
Zn 0.591 0.879 0.531

Zn 0.591 0.712 0.531
Zn 0.288 0.879 0.531
Zn 0.288 0.409 0.531
Zn 0.121 0.712 0.531
Zn 0.121 0.409 0.531
Zn 0.445 0.890 0.501
Zn 0.445 0.555 0.501
Zn 0.110 0.555 0.501
Zn 0.943 0.557 0.499
Zn 0.943 0.386 0.499
Zn 0.614 0.557 0.499
Zn 0.614 0.057 0.499
Zn 0.443 0.386 0.499
Zn 0.443 0.057 0.499
Zn 0.442 0.721 0.499
Zn 0.279 0.721 0.499
Zn 0.279 0.558 0.499
Zn 0.781 0.562 0.496
Zn 0.781 0.219 0.496
Zn 0.438 0.219 0.496
Zn 0.778 0.389 0.491
Zn 0.611 0.389 0.491
Zn 0.611 0.222 0.491
Zn 0.879 0.591 0.031
Zn 0.879 0.288 0.031
Zn 0.712 0.591 0.031
Zn 0.712 0.121 0.031
Zn 0.409 0.288 0.031
Zn 0.409 0.121 0.031
Zn 0.890 0.445 0.001
Zn 0.555 0.445 0.001
Zn 0.555 0.110 0.001
O 0.609 0.888 0.877
O 0.609 0.721 0.877
O 0.279 0.888 0.877
O 0.279 0.391 0.877
O 0.112 0.721 0.877
O 0.112 0.391 0.877
O 0.445 0.890 0.875
O 0.445 0.555 0.875
O 0.110 0.555 0.875
O 0.945 0.556 0.874
O 0.945 0.389 0.874
O 0.611 0.556 0.874
O 0.611 0.055 0.874
O 0.444 0.389 0.874
O 0.444 0.055 0.874
O 0.445 0.723 0.873
O 0.277 0.723 0.873
O 0.277 0.555 0.873
O 0.778 0.556 0.872
O 0.778 0.222 0.872

O 0.444 0.222 0.872
O 0.779 0.389 0.872
O 0.611 0.389 0.872
O 0.611 0.221 0.872
O 0.888 0.609 0.377
O 0.888 0.279 0.377
O 0.721 0.609 0.377
O 0.721 0.112 0.377
O 0.391 0.279 0.377
O 0.391 0.112 0.377
O 0.890 0.445 0.375
O 0.555 0.445 0.375
O 0.555 0.110 0.375
O 0.556 0.945 0.374
O 0.556 0.611 0.374
O 0.389 0.945 0.374
O 0.389 0.444 0.374
O 0.055 0.611 0.374
O 0.055 0.444 0.374
O 0.723 0.445 0.373
O 0.723 0.277 0.373
O 0.555 0.277 0.373
O 0.556 0.778 0.372
O 0.222 0.778 0.372
O 0.222 0.444 0.372
O 0.389 0.779 0.372
O 0.389 0.611 0.372
O 0.221 0.611 0.372

Str 105 (WZ-ZnO-NP-19)
$\Delta E_{gap}(PBE_{GW-fit})$: 0.81 eV
E_{rel}: 0.32 eV/ZnO
$Pore_{max}$: 0.75 nm
V_{pore}: 33 %
D_{pore}: 1
cell parameters
16.419 16.419 5.373 90.00 90.00 120.00
fractional coordinates
Zn 0.667 0.935 0.998
Zn 0.068 0.333 0.998
Zn 0.065 0.932 0.998
Zn 0.868 0.931 0.996
Zn 0.863 0.132 0.996
Zn 0.069 0.137 0.996
Zn 0.951 0.895 0.526
Zn 0.744 0.049 0.526
Zn 0.105 0.256 0.526
Zn 0.940 0.452 0.524
Zn 0.548 0.688 0.524
Zn 0.312 0.060 0.524
Zn 0.933 0.067 0.502
Zn 0.923 0.264 0.501

Zn 0.736 0.859 0.501
Zn 0.141 0.077 0.501
Zn 0.533 0.868 0.498
Zn 0.135 0.467 0.498
Zn 0.132 0.865 0.498
Zn 0.337 0.869 0.496
Zn 0.332 0.663 0.496
Zn 0.131 0.668 0.496
Zn 0.456 0.905 0.026
Zn 0.249 0.544 0.026
Zn 0.095 0.751 0.026
Zn 0.888 0.348 0.024
Zn 0.652 0.740 0.024
Zn 0.260 0.112 0.024
Zn 0.267 0.733 0.003
Zn 0.464 0.723 0.001
Zn 0.277 0.941 0.001
Zn 0.059 0.536 0.001
O 0.933 0.067 0.875
O 0.930 0.266 0.873
O 0.734 0.864 0.873
O 0.136 0.070 0.873
O 0.534 0.861 0.872
O 0.139 0.872 0.872
O 0.128 0.466 0.872
O 0.334 0.866 0.872
O 0.332 0.666 0.872
O 0.134 0.668 0.872
O 0.938 0.872 0.871
O 0.734 0.062 0.871
O 0.128 0.266 0.871
O 0.931 0.467 0.869
O 0.533 0.664 0.869
O 0.336 0.069 0.869
O 0.267 0.733 0.375
O 0.466 0.730 0.373
O 0.270 0.936 0.373
O 0.064 0.534 0.373
O 0.666 0.928 0.372
O 0.072 0.939 0.372
O 0.061 0.334 0.372
O 0.868 0.934 0.372
O 0.866 0.132 0.372
O 0.066 0.134 0.372
O 0.466 0.928 0.371
O 0.262 0.534 0.371
O 0.072 0.738 0.371
O 0.864 0.333 0.369
O 0.667 0.731 0.369
O 0.269 0.136 0.369