University of Tehran
Department of Physics

Mass Transport through Nano-Structured Membranes

By: Khatereh Azizi

Under Supervision of Dr. Seyed Mehdi Vaez Allaei
and Advice of Dr. Tapio Ala-Nissila

A thesis submitted to the Graduate Studies Office
In partial fulfillment of the requirements for
The degree of PhD in

Solid State Physics

September 2021

Abstract

Transport of a fluid through a membrane has always been an important problem to the study, especially when it is in the nano-scale having unique as well as diverse properties. In studying transport, one also needs to look at the fluid features in the vicinity of the membrane. These two problems are completely related to each other and we will go through both in the thesis. Regarding this, we have studied two different systems: first, fluid of gas molecules in the vicinity of graphyne-3, as well as their transports though that, second, water at the the interface of neutral and charged amorphous silica as the first step of investigating the water transport through a silica channel.

In the first system, we studied the small gas molecules (H_2,CO_2, CH_4, and C_2H_6) in the vicinity of graphyne-3, as well as looking at the transport of gaseous mixtures through the membrane and their separation, yielding to consistent results. We also studied the effect of pressure the difference, the concentration of the molecules, and the scalability of the results, which showed that the permeability is independent to the pressure difference and the system size (hence it is scalable), and it changes linearly as a function of concentration. The other an important property is the thermal fluctuations of the membrane, which affects the results considerably, something usually ignored by people in other studies. One of the most important results is the high the permeance of gases, together with a good separation factor, which are due to the 2D structure of graphyne-3, intrinsic nano-pores in the size of the van der Waals radii of gases, and the type of the interaction between gases and the membrane. We also showed that graphyne-3 is much better than any other studied membranes in the separation of carbon dioxide and ethane.

Regarding the water-silica system, we studied the static and dynamic properties of water near both the neutral and charged silica surface. We observed that the static properties do not change so much due to the surface charge, while the dynamic properties are affected a lot in a way that the water near the charged silica surface becomes less dynamic. The friction between water and silica has also been studied and shows a 10-order of magnitude enhancement of friction coefficient due to the surface charge. This thesis is going to be followed by water transport through a silica channel in the near future.

In addition, we assigned some part of the thesis to the LAMMPS modification of having the three-body potential describing the silica the surface at the interface. We have developed the code and it is simply usable like other potentials in the LAMMPS package.

All in all, we studied the 2-D and 3-D membranes in the nano-scale and the fluids (gas and water) near that. We observed that the properties of the system and the transport is fully related to the dynamic properties of the fluid near the membrane. Also, in the nano-scale, the system will have unique features, e.g. very large permeability of gas molecules through the graphyne-3 membrane, and a very large friction between water and amorphous silica. In summary, with studying the transport through nano-structures, one can gain many interesting knowledge around the physical properties, as well as knowing diverse applications of the system.

Keywords: Transport, Graphyne-3, Gas Separation, Silica, Friction, Interface Properties