Supplementary Material (ESI) for PCCP

"Salt parameterization can drastically affect the results from classical atomistic simulations of water desalination by MoS_2 nanopores"

João P. K. Abal[‡,a], José Rafael Bordin[†,b] and Marcia C. Barbosa[‡,c]

‡*Institute of Physics, Federal University of Rio Grande do Sul, Brazil*

†*Department of Physics, Institute of Physics and Mathematics, Federal University of Pelotas, Brazil.*

[a] joao.abal@ufrgs.br [b] jrbordin@ufpel.edu.br [c] marcia.barbosa@ufrgs.br

Water Flux Comparison

The results for the combination of narrow nanopore and TIP4P/2005 + NaCl/J obtained in this work are comparable to the ones obtained by Reference [1]. The comparison are presented in the following water flux graph (Figure 1). The pore area (Figure 2) was obtained following the Reference [1] recipe, in which consists of using the van der Waals radii of sulfur and molybdenum.

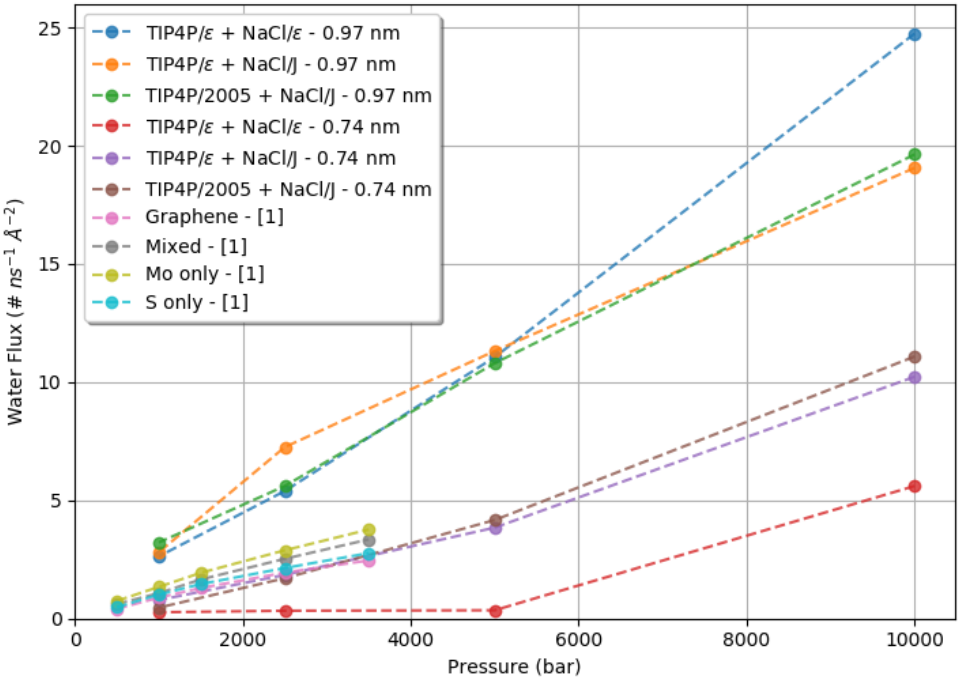

FIG. 1. The membrane water flux for distinct combinations of water and salt models (this work), with the Reference [1] comparison.

For the comparison, the three MoS_2 pores and the graphene pore have approximately equivalent accessible pore areas (mixed - 55.45 $\AA^2$; Mo only - 56.42 $\AA^2$; S only - 57.38 $\AA^2$; and graphene - 59.67 $\AA^2$. Reference [1]).

As we can see in Figure 1, the combination of TIP4P/2005 + NaCl/J + mixed 34.39 $\AA^2$ of nanopore area (this work) and SPC/F + NaCl/J + mixed 55.45 $\AA^2$ of nanopore area (Reference [1]) lead to similar water fluxes as well as negligible ion blocking effect.

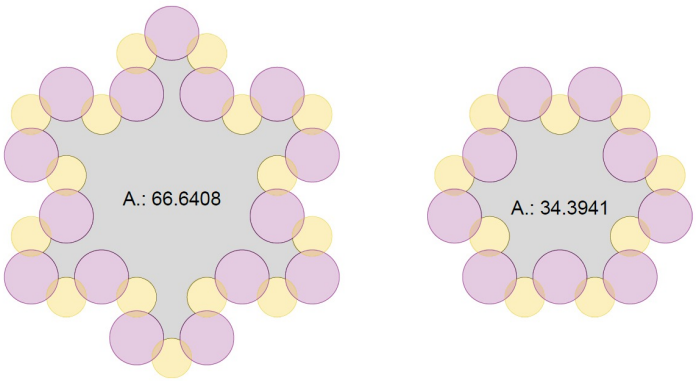

FIG. 2. The pore area was obtained by computing the accessible area to water molecules considering the size of the atoms on the edge of each pore as the van der Waals radii of sulfur and molybdenum as inputs. This procedure follows the Reference [1].

The Charge Distribution Comparsion - preliminary study

The charges affects the water transport by attracting or repelling the water molecules depending on the nanopore region. The Mo atoms attract the oxygen although the S atoms attracts the hydrogen atoms. The water molecules can assume different density distributions depending on the charge distribution as well. As a consequence, the total effective space, in which the water molecules could use to pass through the nanopore, is different for each charge distribution (Reference [1]).

In order to evaluate this effect, we have performed a very preliminary study, which is not the main focus of this paper, in which we compare the water inside a MoS_2 pore with and without the electrostatic interactions. No electrostatic interactions means that the membrane interact with other particles just with the Lennard-Jones potential. This simulation was carried with a pressure gradient of 1000 bar at 300 K.

The results are summarized as follows. In Figure 3-(a), the filtered water molecules per time are shown for the case in which the nanopore interact also throught coulombic forces (called "Coulombic Nanopore") and for the case in which the nanopore interact only through Lennard-Jones (called "LJ Nanopore"). As we can see, the presence of the charges in the neutral system affects the overall water flux. Also the charge distribution has implications in the hydrogen-bonding network (HB) around the nanopore: the mean HB number per water molecule is higher for the LJ Nanopore case,

as shown in Figure 3-(b). The Figures 3-(c)-(d) shows how the water molecules assume different density distributions inside the nanopore depending on each case.

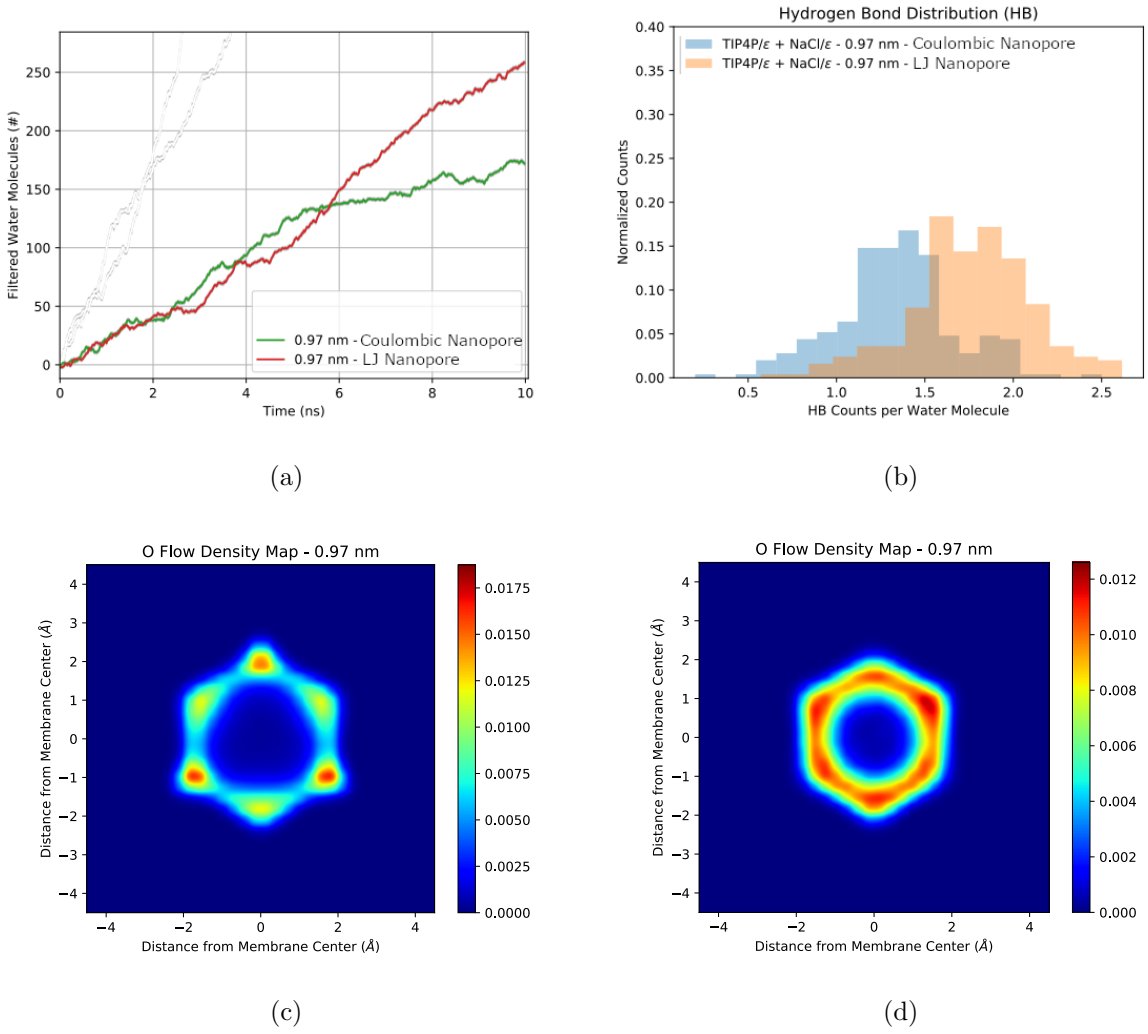

FIG. 3. The so called "Coulombic Nanopore" is referent to the case in which the particles interact with the nanopore via the LJ and Coulomb interactions. The so called "LJ Nanopore" is referent to the case in which the particles interact with the nanopore only via the LJ interaction. (a) The filtered water molecules per time are shown for the two cases. (b) The Hydrogen-Bonding number per water molecule distribution inside and around the nanopore are shown for the two cases. (c) The Oxygen flow density map for the "Coulombic Nanopore" case. (d) The Oxygen flow density map for the "LJ Nanopore" case.

Hence, the charge distribution affects the overall membrane performance. In addition, the two MoS_2 structures studied, although represents different charge distributions, are symmetric once it

preserves the proportion between the Mo and S stoichiometry. So, the overall net attraction or repulsion is the same for both cases.

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[1] M. Heiranian, A. B. Farimani and N. R. Aluru, *Nature Communications*, 2015, **6**, 8616.