Application of the Tight Binding GFN2-xTB Method to Model Large Interstellar Amorphous Icy Grains

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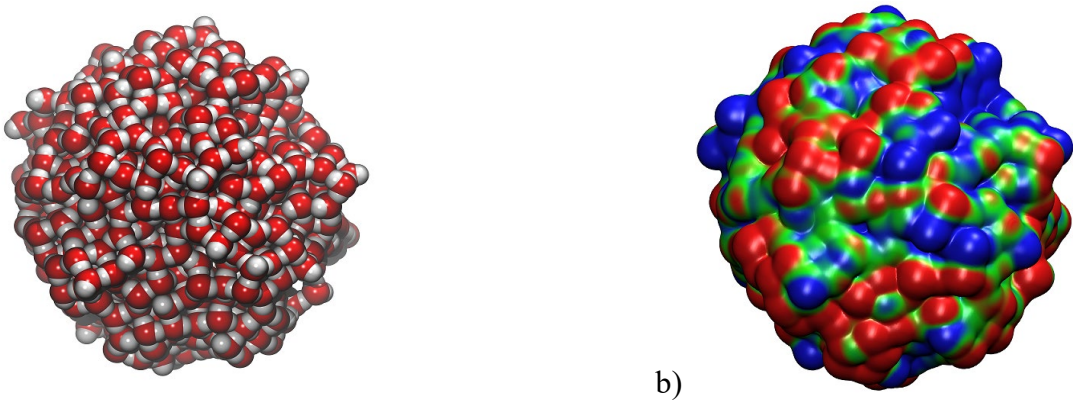
Interstellar grains are made of a silicate core covered by a mantle of several layers of amorphous ice. In the gas-phase of dense molecular clouds chemical species freeze onto the grain and can diffuse on its surface, react to give interstellar more complex molecules and ultimately desorb back to the gas-phase. Hence, the study of interstellar grains is an important part for understanding the chemical evolution in time of the Interstellar Medium (ISM). There is still no consensus in the Astrochemistry community on how to model these icy grains at atomistic level with the requisite of treating the hydrogen bond interaction and other important components accurately. Furthermore, the grain should be large enough to be representative of the variability present in the ISM, which renders impractical the adoption of plain DFT methods. Also, the adopted method should, not only be relatively fast, but also applicable to study the interaction of large interstellar molecules with the grain itself. Force fields are not the proper solution, due to the parametrization specific for each considered species, breaking the universality of the approach. To fill in the above requested, we resort to a newly developed semi-empirical quantum mechanical method based on the tight binding DFT approach called GFN2-xTB[1] and a universal force field method called GFN-FF[2], both developed by the Grimme's group at the Bonn University. We present the methodology to build a water cluster model up to 1000 H2O molecules and to characterize its structural and electrostatic potential surface (EPS) as a free grain (Fig. 1). Then, NH3 was chosen as relevant interstellar molecule to compute its binding energy (BE) at more than 150 different grain sites to characterize the BE distribution which revealed a bimodal distribution.



a) b)

Figure 1: a) Structure and b) EPS of the GFN2-xTB water cluster model (1000 H2O)

References

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[2] S. Spicher, S. Grimme, Angew. Chem. Int. Ed. 2020, 59, 15665-15673