Advances and Challenges in Modeling Water Clusters and Liquid Water

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Understanding the properties of water, in its various phases and at different interfaces, is a key subject in numerous chemical, physical, and biological processes.[1] This is evidenced through the numerous experimental and theoretical studies on water that have been published over the past decades. In the latter cases, despite its simple molecular structure, accurately modelling water remains a significant challenge due to its complex hydrogen-bonding network and the nuclear quantum effects that influence its behaviour.[2]

In this presentation, I will discuss recent advancements in the theoretical modelling of water clusters and liquid water conducted at the LCPQ (Laboratory of Quantum Chemistry and Quantum Physics). Emphasis will be placed on the methodologies employed, including self-consistent-charge density-functional based tight-binding (SCC-DFTB) formalism [3], molecular dynamics and path-integral molecular dynamics approaches,[4] and enhanced sampling methods. I will highlight the benefits and limitations of these approaches, particularly focusing on the issues of sampling of potential energy surfaces and inclusion of nuclear quantum effects (NQEs). Additionally, I will present recent studies from our group at LCPQ, showcasing our efforts in enhancing the accuracy of water models. Finally, I will explore the potential of Machine Learning (ML) tools to improve the modelling of water.

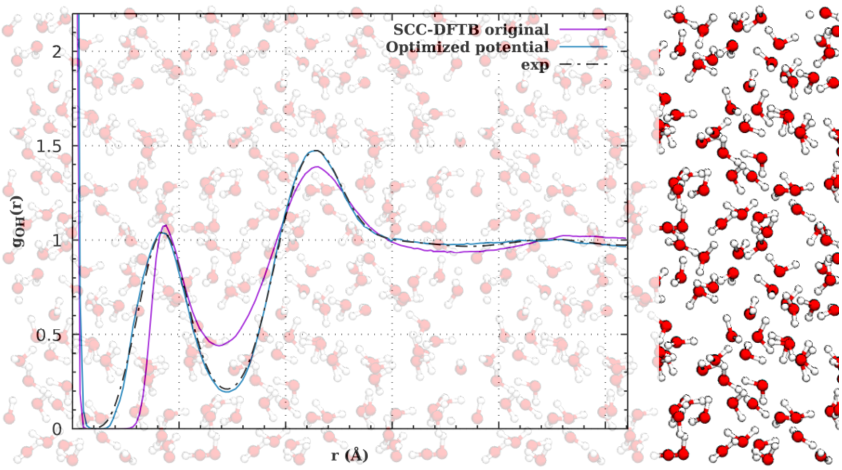

Figure 1: O-H pair radial distribution function of liquid water obtained from the original and optimized SCC-DFTB potentials as compared to the experimental curve.

Keywords: Aqueous Systems, Molecular Dynamics, Enhanced Sampling, Machine Learning.

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