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An analysis of the structural and dynamic properties of flexible water models

Life cannot exist or evolve without liquid water, which is a substance composed of a molecule that is both simple and complicated to understand. In Latin, it is called “Aqua via”. Water is a universal solvent because of its polarity and hydrogen bonds, which allow many chemical substances such as salts and ions to dissolve. Therefore, water models are studied to simulate its structural and thermodynamic properties in biological systems and biochemistry. In this study, we have simulated some flexible water models for environmental applications. By introducing flexible O-H bonds and H-O-H angles, modeled as springs oscillating around an equilibrium length or angle, we were able to improve the dynamic and structural properties of water models such as the diffusion coefficient, vibration spectrum, dielectric constant, density, and Radial Distribution Function. There are different types of water models classified according to the number of interaction sites, and we have used some of them in this study (SPC/E [1], TIP3PFw [2], mSPCFw [3], OPC3 [4], TIP4P [5], TIP4PEw [6], TIP4P2005f [7], OPC [8]) [9-10]. It is worth noting that each of these models has been configured for a specific application. The results obtained and compared on some structural and dynamic properties of the different models used are presented in Figure 1a, 1b, and 1c. Among all the models chosen, we were able to obtain two models that were able to reproduce all the properties of water in this study, which are TIP4P/2005f and SPC/E.

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