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Adiabatic Intramolecular Movements for Water Systems in Ab initio simulations[1] LUANA PEDROZA, ANTONIO J.R. DA SILVA, Physics Institute USP — The detailed description of hydrogen bonds in water is essential to understand the great variety of processes that occur in this system. Clearly the most appropriate way to do that description would be to treat all the degrees of freedom quantum mechanically. Another possibility is to treat the nuclei classically and the electrons quantum mechanically. A very commom approximation in these simulations is to consider each water molecule as a rigid body, which clearly imposes a limitation on the real description of the molecules and their interactions. We here present an effective treatment of the intramolecular degrees of freedom of water, where these modes are decoupled from the intermolecular one, adiabatically allowing these coordinates to be positioned at their local minimum of the PES. This decoupling is performed combining an AIMC simulation using the rigid bodies approximation with an intramolecular optimization. As an application of our methodology we have studied small water clusters. We show that even in the case of the water dimer the sampling of phase space is significantly modified when intramolecular optimization is included (J. Chem. Phys., 128, 104311 (2008)). As a result, there are clear changes in features such as the dipole moment and structural properties.

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