LOW-FREQUENCY INFRARED SPECTRUM OF LIQUID WATER FROM MACHINE-LEARNING BASED PARTIAL ATOMIC CHARGES

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Modeling water in condensed phases is an indispensable part of modern water research and rigid non-polarizable water models, such as TIP4P/2005, have been very popular in molecular simulations due to their high efficiency. Although these water models can reproduce many properties of water, they fail in predicting the dielectric properties of water, such as the dielectric constant and low-frequency infrared spectra. We propose to improve these models by re-assigning the partial atomic charges of water molecules according to their local environment using a machine-learning (ML) model that is trained on quantum chemical data. With the ML-based charges, the calculated low-frequency infrared spectrum of liquid water is in good agreement with experiment, showing a peak at about 200 cm^{-1}, which non-polarizable water models fail to reproduce. The effects of charge redistributions in liquid water and their dependence on the choice of the density functional are also discussed.