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Structural, Dynamic, and Spectroscopic Properties of the SCC-DFTB Water Model LAURA KINNAMAN, KATHIE NEWMAN, STEVEN CORCELLI, University of Notre Dame — The interactions of water and many interfaces are not understood at a mechanistic level. The accuracy of simulations of the system are limited by the accuracy of the water model used. Classical models such as SPC/E use empirically derived parameters to match their behavior to desired bulk water properties, but cannot participate in reactions that require the making or breaking of bonds. Ab initio quantum mechanical methods such as Car-Parrinello (CP) do allow water to dissociate, but are computational intractable for large systems. A potential middle ground is the self-consistent charge density-functional tight-binding method (SCC-DFTB), which has a smaller associated computational cost, and therefore can access larger systems than CP, while still allowing for the making and breaking of bonds. The DFTB+ implementation of SCC-DFTB allows for 2nd and 3rd order expansions of the density fluctuations in the energy and, in the 3rd order expansion, an optional damping correction factor. For each of these models we compare the structural, dynamic, and spectroscopic properties of bulk SCC-DFTB water to classical SPC/E and experimental results.

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