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Hamiltonian QM/MM scheme based on a plane-wave DFT approach ANGELO BONGIORNO, SEUNG BUM SUH, ROBERT BARNETT, UZI LANDMAN, Georgia Institute of Technology, School of Physics, Atlanta, Georgia 30332-0430 — We present an Hamiltonian quantum mechanical (QM)/molecular mechanical (MM), QM/MM, scheme for investigating large biological systems. The QM region is described through a plane-wave density-functional theory approach, while for the MM region we use the AMBER force field. The QM and MM regions are merged in our scheme across C-C bonds. These bonds are saturated by using hydrogen-like pseudopotentials. Charge consistency across the QM/MM interface is achieved by generating norm-conserving pseudopotentials accounting for the values of the MM effective charge. The interaction between the QM region and non-bonded MM ions includes van der Waals and coulomb interactions. Spill-out effects and spurious large electrostatic interactions at the frontier between the QM and MM regions are avoided by smearing the MM effective ionic charges according to a gaussian distribution. Our QM/MM scheme well reproduces the properties of the water dimer, water, small organic molecules, and large oligomers, as compared to either full MM and QM calculations.

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