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Hybrid DFT/Thomas-Fermi simulations and applications to biological systems MIROSLAV HODAK, North Carolina State University, Raleigh, WENCHANG LU, JERRY BERNHOLC — We have developped a hybrid simulation method suitable for performing calculations on biological systems. Within this method, Density Functional Theory (DFT) is used for the chemically active region and some solvent molecules, while the rest of the solvent molecules are treated with a variant of Thomas-Fermi (TF) theory, which uses the generalized gradient approximation (GGA) kinetic energy functional. These TF solvent molecules are assumed to be rigid and have frozen electron densities, which allows for their efficient treatment. Both Kleinman-Bylander and ultrasoft types of pseudopotentials are implemented within our method. We find it efficient to first equilibriate bio-molecules in solvent environment using classical molecular dynamics. After the initial equilibriation we use the hybrid method to study chemical reactions involving the bio-molecule. Initial applications to transition metal ions-protein complexes in solution will be discussed.

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