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Hybrid DFT/Thomas-Fermi-like simulations of solvated molecules in water MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, Raleigh — We have developed a hybrid method for efficient and accurate treatment of systems that involve a chemically active part surrounded by a large number of solvent molecules. The chemically active region is treated with Density Functional Theory (DFT), while most of the solvent molecules are treated with a variant of Thomas-Fermi (TF) theory, in which the TF kinetic energy functional was replaced by one based on the generalized gradient approximation (GGA). These solvent molecules are also assumed to be rigid and have frozen electron densities. The exchange of solvent molecules between the two regions is allowed as is the overlap of densities. We show that the calculation in which small mumber of water molecules is treated with DFT, while the TF-like approach is used for most of the molecules, leads to a good description of the entire water system. This calculation takes only a fraction of computer time required for a full DFT treatment of the whole system. Initial applications to biological systems will also be discussed.

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