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Complex wet-environments in electronic-structure calculations[1]
GIUSEPPE FISICARO, University of Basel, LUIGI GENOVESE, Laboratoire de simulation atomistique (L-Sim), SP2M, INAC, CEA-UJF, OLIVIERO ANDREUSSI, Institute of Computational Science, Universitá della Svizzera Italiana & THEOS-MARVEL École Polytechnique Fédérale de Lausanne, NICOLA MARZARI, THEOS-MARVEL École Polytechnique Fédérale de Lausanne, STEFAN GOEDECKER, University of Basel — The computational study of chemical reactions in complex, wet environments is critical for applications in many fields. It is often essential to study chemical reactions in the presence of an applied electrochemical potentials, including complex electrostatic screening coming from the solvent. In the present work we present a solver to handle both the Generalized Poisson and the Poisson-Boltzmann equation. A preconditioned conjugate gradient (PCG) method has been implemented for the Generalized Poisson and the linear regime of the Poisson-Boltzmann, allowing to solve iteratively the minimization problem with some ten iterations. On the other hand, a self-consistent procedure enables us to solve the Poisson-Boltzmann problem. The algorithms take advantage of a preconditioning procedure based on the BigDFT Poisson solver for the standard Poisson equation. They exhibit very high accuracy and parallel efficiency, and allow different boundary conditions, including surfaces. The solver has been integrated into the BigDFT and Quantum-ESPRESSO electronic-structure packages and it will be released as a independent program, suitable for integration in other codes. We present test calculations for large proteins to demonstrate efficiency and performances.

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