

Supplementary Information: Inertial Extended-Lagrangian Scheme for Solving Charge Equilibration Models

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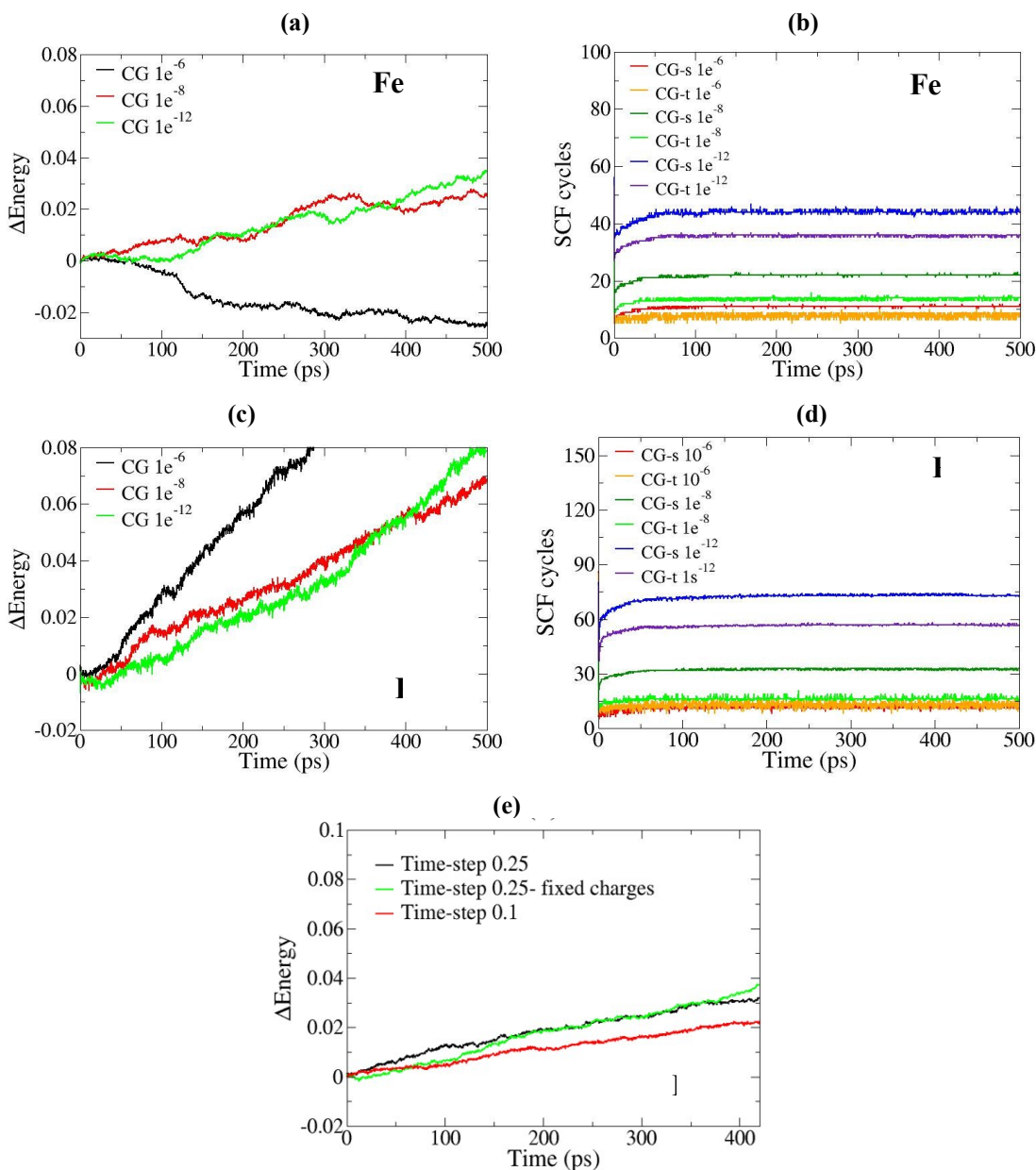


Figure S1. Comparison of energy conservation and number of SCF cycles using the standard CG-SCF solution at different convergence tolerances for charge equilibration. Energy conservation of CG-SCF at 10^{-6} , 10^{-8} , 10^{-12} level of convergence for (a) FeOH₃ and (c) RDX. Number of SCF cycles required to reach convergence at 10^{-6} , 10^{-8} , 10^{-12} for q_{SCF}^s and q_{SCF}^t for (b) FeOH₃ and (d) RDX. (e) Energy dissipation analysis for the HNS system at a convergence tolerance of 10^{-8}