Calculation of redox potentials for iron-sulfur proteins

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Metalloproteins are key components to energy transduction in several biochemical pathways through redox reactions. Here, we investigate isolated models of iron-sulfur cofactors and a simple protein, rubredoxin, in an all-atom framework to identify the main physical contributions to the calculation of redox potentials employing QM/MM hybrid methods. Calculations in an ionic force (salt, NaCl) setup presented poor convergence due the challenging sampling of ion configurations. A proper description of the polarization around the redox center is required and demands a large quantum region of up to 200 atoms around the central iron-sulfur center. Finite model effects, level of quantum-mechanical treatment, explicit hydration of cofactors and configurational sampling were also evaluated.