Poster presentation

Computation of accurate redox potentials for Fe, Mn and Ni model complexes

A Galstyan* and EW Knapp

Address: Free University of Berlin, Institute of Chemistry and Biochemistry, Fabeckstr. 36a, D-14195 Berlin, Germany

* Corresponding author

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A combination of density functional theory (DFT) and solution of the Poisson equation for continuum dielectric media was used to compute accurate redox potentials for several mononuclear transition metal complexes including iron, manganese and nickel. Progress was achieved by altering the B3LYP DFT functional (B4(XQ3)LYP-approach) and supplementing it with an empirical correction term, which is applied after the quantum-chemical DFT computations. Calculation of the 58 redox potentials of 48 different transition metal complexes shows a root mean square deviation from experimental values of 65 mV. The quality of the present approach becomes also evident by observing that the energetic order of the spin multiplicity is fulfilled for all considered transition metal complexes. For some transition metal complexes it was necessary to account for the dielectric environment before agreement with the corresponding measured spin multiplicities was obtained.