Development and Application of Oxidation-State Constrained Density Functional Theory (OS-CDFT) for Quantitative Description of Electron Transfer Problems

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Electron transfer is a fundamental and ubiquitous process in biology and in many applications like molecular electronics as well as energy harvesting and storage. Quantitative description of electron transfer processes through simulations requires accrate generation of the diabatic states to determine the key parameters like the energy of reaction, the reorganization energies and the transfer matrix. Here, I will present the development of the oxidation-state constrained density functional theory (OS-CDFT) approach for effective generation of the diabatic states and study of electron transfer processes.[1] Unlike conventional constrained DFT, OS-CDFT controls directly the oxidation states of transition metal ions basing on the unambiguous approach for determination of the oxidation states.[2] After discussion of the methodology development, I will highlight its applications to various electron transfer problems including polaron dynmics in transition metal compounds and accurate bandgap calculations.[3,4,5]

References

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