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Building Molecular Modeling Strategy: Charge Response Kernel Comprising Density Functional Theory and the Treatment of Conformational Effect on it

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For constructing molecular modeling strategy considering polarization effects, we have proposed an extended treatment of the charge response kernel (CRK), which describes the response of partial charges on atomic sites to external electrostatic potential, $K_{ab} = \partial Q_a / \partial V_b$, where Q_a represents the partial charge at the site a and V_b stands for the electrostatic potential at the site b, on the basis of the density functional theory (DFT) via the coupled perturbed Kohn-Sham equations. The present CRK theory incorporates charge regulation procedures with a reliable warranty in the definition of partial charges to avoid unphysical large fluctuation of the CRK on “buried” sites. Also, it was shown that the improvement of the performance from the calculation results of polarizabilities with the CRKs for methanol, ethanol, propanol, butanol, dimethylsulfoxide (DMSO) and tetrahydrofuran (THF) was achieved, comparing with experimental results.[1] The present CRK model is now extended to investigate optimal partial charges and CRKs available for the systems which conformational changes can be expected by introducing a fitting method in least-square sense to estimate partial charges and CRKs with the data collected from conformational space sampling. We will show our fitting scheme is available for building molecular modeling considering polarization effect explicitly even in the case that target systems include a lot of conformers. [2]

[1] T. Ishida and A. Morita, J. Chem. Phys., **125**, 074112 (2006)

[2] T. Ishida and A. Morita, in preparation