Systematic Evaluation of Reaction Field Schemes for Coupling COSMO Polarizable Continuum Model and Second-order Wavefunction Methods for Computing Solvatochromic Shift

Sarah Karbalaei Khani and Christof Hättig[a]

[a] Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D–44780 Bochum, Germany
sarah.karbalaeikhani@rub.de

A reaction field is an electrostatic field G[D] generated from the interaction of the solute charge distribution D and a polarizable environment. For post-HF methods, various schemes have been introduced to describe the interaction between the correlated part of the wavefunction of the QM system and the polarizable environment. In this study, the assessment of three reaction field schemes, including the perturbation on the energy-only scheme (PTE), the iterative perturbation on the energy and density scheme (PTED) and the post-SCF scheme, Fig. 1, were considered for the calculation of solvatochromic shifts. We composed two benchmark data sets and compared the solvatochromic shifts resulted from the experiment and theory.

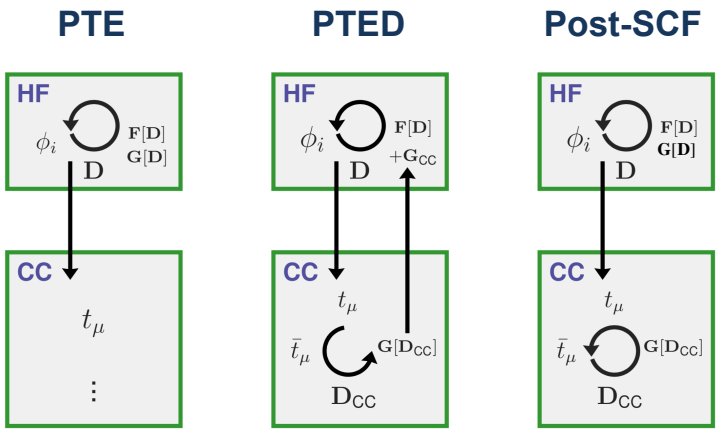

Figure 1: Reaction field schemes in coupled cluster theory.

References

1. B. Lunkenheimer and A. Köhn, J. *Chem. Theory Comput.* **9** (2013), 977.
2. T. Schwabe, K. Sneskov, J. M. Olsen, J. Kongstad, O. Christiansen and C. Hättig, J. *Chem. Theory Comput.* **8** (2012), 3274.