Electronic structure of species in condensed matter environment from frozen-density embedding theory based simulations

T.A. Wesolowski

1. *Department of Physical Chemistry,University of Geneva, 30, quai Ernest-Ansermet*, *CH-1211*

Frozen-Density Embedding Theory (FDET) [1,2,3] is a variational-principle based general formal framework, which uses the charge density as the only descriptor for the environment of an embedded species. It yields an optimal embedded wavefunction for evaluation of quantum-mechanical observables (excitation energies, NMR parameters, polarizabilities, etc.). The electron density of the environment (ρ_B), used in such calculations can be obtained using various methods: from lower level quantum mechanical calculations [6-7], continuum models [4-5], or even experiment. In the first part, we will provide a few examples of such simulations. In the second part, we will overview the sensitivity of the FDET results to variations of ρ_B [8,9].

Acknowledgments: This research has been supported by Swiss National Science Foundation (200021-152779)

References:

[1] T.A. Wesolowski & A. Warshel, J. Phys. Chem, **Vol. 97** (1993) 8050
[2] T.A. Wesolowski, Phys. Rev. A., **Vol. 77** (2008) 012504
[3] T.A. Wesolowski J. Chem. Phys. **Vol. 140** (2014) 18A530
[4] X. Zhou, J.W. Kaminski, T.A. Wesolowski, Phys. Chem. Chem. Phys., **Vol. 13** (2011) 10565
[5] S. Shedge & T.A. Wesolowski, (2014) to be published
[6] X. Zhou, T.A. Wesolowski, G. Tabacchi, E. Fois, G. Calzaferri, A. Devaux, Phys. Chem. Chem. Phys, **Vol. 15**, (2013) 159
[7] X. Zhou, D. Sundholm, T.A. Wesolowski, V.R.I Kaila, J. Am. Chem. Soc. **Vol. 136**, (2014) 2723
[8] M. Humbert-Droz, S.S. Shedge, X. Zhou, T.A. Wesolowski, Theor. Chem. Accounts. **Vol. 132**, (2013) 1405
[9] A. Zech, F. Aquilante & T.A. Wesolowski (2015) to be published