Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Charge Transfer Couplings and Excitation Energies From Subsystem DFT: The Ultimate Divide and Conquer Approach to DFT MICHELE PAVANELLO, Rutgers University — The subsystem formulation of DFT known as Frozen Density Embedding (FDE) offers an excellent platform for studying charge transfer reactions in solvated systems, such as biosystems. I present new theory and software development for the calculation of the electronic couplings as well as the charge transfer excitations from FDE derived densities. The method presented scales linearly with the number of non-covalently bound subsystems considered in the calculation. Proof-of-principle calculations of water and ethylene clusters with up to 56 monomers are presented. In addition, DNA oligomers radical cations, including donor-acceptor, donor-bridge-acceptor, as well as a prototype of the phothosynthetic reaction center are tackled and preliminary results are presented.

Michele Pavanello
Rutgers University

Date submitted: 29 Nov 2012 Electronic form version 1.4