THEOS
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QM/classical approaches to model environment effects in electronic energy transfer processes

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Abstract: Photon absorption and electronic energy transfer (EET) represent the first processes in both natural and artificial light-harvesting systems. In the pursuit of mimicking the optimal design of natural light-harvesting antennae it is of fundamental importance to achieve a molecular-level explanation of these processes and the way they are affected by the environment [1]. Such a goal is formidably challenging due to the large network of interactions that couple all the parts of the system and the different time and length scales involved. However, a possible strategy exists and it is represented by the coupling of quantum chemical methods to classical approaches that account for the environment response in all the steps of the process. Two alternative classical approaches are here presented and discussed, namely a continuum model [2] and a MM force field [3]. In both cases explicit treatment of the environment polarization is introduced.

[1] B. Mennucci, C. Curutchet, Phys. Chem. Chem. Phys., 13 (2011) 11538.
[2] M.F. Iozzi, B. Mennucci, J. Tomasi, R. Cammi, J. Chem. Phys., 120 (2004) 7029.
[3] C. Curutchet, A. Munoz-Losa, S. Monti, J. Kongsted, G. D. Scholes, B. Mennucci, J. Chem. Theory Comput., 5, (2009) 1838.