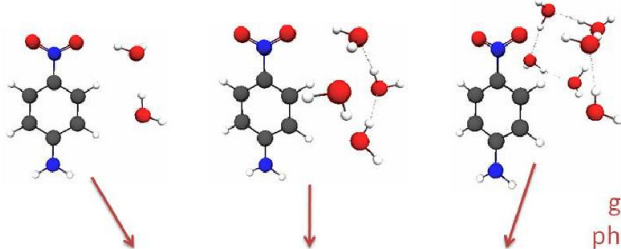


What's New in Q-Chem

EOM-CC/EFP for the Electronically Excited and Ionized States

Developers: Lyudmila Slipchenko

A combination of EFP with CCSD and EOM-CCSD methods offers a unique tool for calculations of electronically excited and ionized states in solutions. In this hybrid approach, the EOM-CC methods are used to describe the QM region (e.g., a chromophore) and EFP describes the MM part (solvent). Different variants of EOM-CC (EE, SF, IP, EA) can be employed allow Q-Chem users to compute a variety of open-shell wave functions in in the condensed phase. CIS, CIS(D), SOS-CIS(D), and TD-DFT methods can also be used in the QM part.



				gas phase:
Full EOM-CCSD:	-0.28 eV	-0.19 eV	-0.26 eV	
EOM-CCSD/EFP:	-0.27 eV	-0.19 eV	-0.24 eV	4.65 eV
Full CIS(D):	-0.33 eV	-0.23 eV	-0.31 eV	4.65 eV
CIS(D)/EFP:	-0.32 eV	-0.22 eV	-0.28 eV	

Solvatochromic shifts in small complexes of p-nitroaniline (pNA) with water calculated with EOM-CCSD/EFP and full EOM-CCSD, and CIS(D)/EFP and full CIS(D). In hybrid QM/EFP calculations pNA is treated with EOM-CCSD or CIS(D), while all waters are represented by EFP. The largest discrepancy between fully quantum and QM/EFP solvatochromic shifts is 0.03 eV. The cost of such QM/EFP calculations is the same as the cost of the respective QM calculation in the gas phase.

For more new features, visit: www.q-chem.com/whatsNew4.html

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