What's New in Q-Chem

Short-Range Corrected Functional for the Calculation of Core-Excited States

Developers: Nick Besley

This feature's functionals introduce a high fraction at very short range in the evaluation of the exchange energy, resulting in considerably more accurate core-excitation energies. The calculation of core excitation energies with time-dependent density functionals in conjunction with standard hybrid functionals normally results in a large underestimation of the excitation energy. This feature is particularly effective for the calculation of core-excited states and NEXAFS spectra with time-dependent density functional.

Nick Besley

Publications:

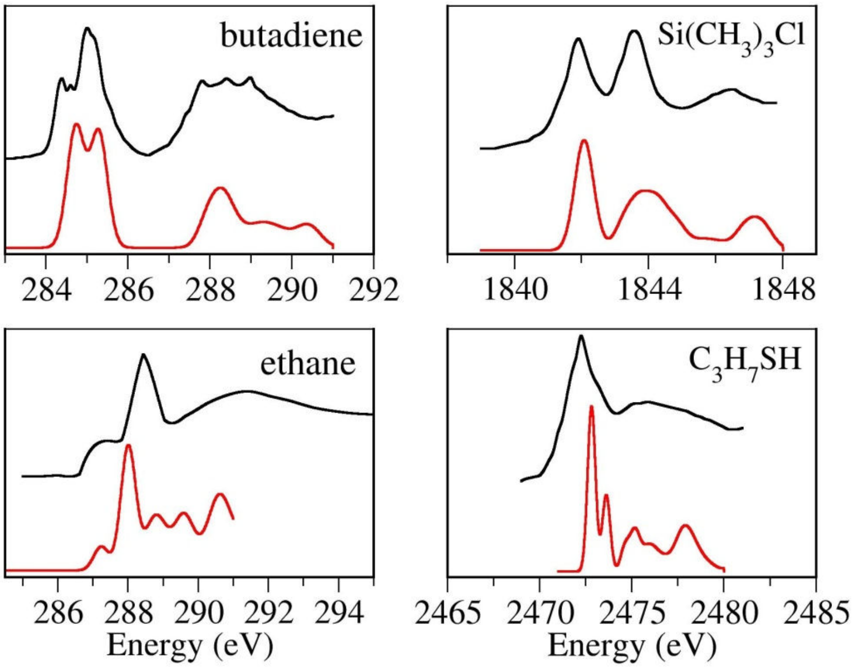
N. Besley, M. Peach, D. Tozer, "Time-dependent density functional theory calculations of near-edge X-ray absorption fine structure with short-range corrected functionals." *Phys. Chem. Chem. Phys.*, **11**, 10350-10358 (2009)

N.A. Besley and F.A. Asmuruf, "Time dependent density functional theory calculations of core electron spectroscopy." *Phys. Chem. Chem. Phys.*, **12**, 12024-12039 (2010)

What’s New in Q-Chem

Short-Range Corrected Functional for the Calculation of Core-Excited States (continued)

The picture shows computed (red line) and experimental (black line) NEXAFS spectra. There is good agreement with experiment and it is not necessary to apply a shift to the calculated spectra.



For more information on how to use this feature, refer to the Q-Chem Manual, Section :
For see more new features, visit: www.q-chem.com/whatsNew4.html