Tuning and spectroscopy of the hydrated electron

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The hydrated electron is a ubiquitous species in aqueous radiation chemistry.
Although known to exist for over 50 years, the microscopic structure of this elusive species was discussed controversially in recent literature.
With ab initio molecular dynamic simulations we could show that the hydrated electron can be pictured as partially similar to a halide ion, localized in a solvent cavity formed by water molecules, but also with a significant part of the hydrated electron delocalized up into the second solvent shell.
These studies and their results are consolidated by comparison to experimental observables like the optical absorption, photoelectron, and the vibrational spectrum.

All these structural, dynamical, or spectroscopic investigations need a solid theoretical foundation and in this talk we will thus focus on the more methodological aspects behind our calculations.
We will take a closer at how density functional theory can be tuned in a systematic manner and how the resulting methodology is able to reproduce experimental observables in a quantitative fashion.

References:
F. Uhlig, O. Marsalek, P. Jungwirth, J. Phys. Chem. Lett. 4, 338 (2013) J. Savolainen, F. Uhlig, S. Ahmed, P. Hamm, P. Jungwirth, Nature Chem. 6, 697
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