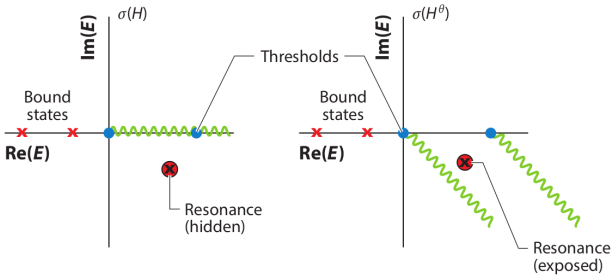
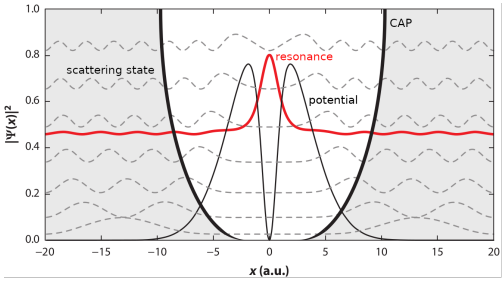
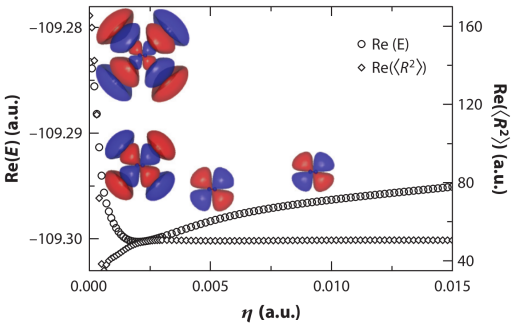
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Calculating Electronic Resonances with Complex-Valued EOM-CC Methods

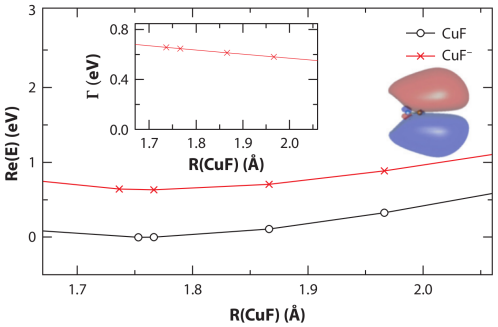




- Resonances are electronically unbound states; they are metastable and decay by ejecting an electron.
- Resonances are embedded in the continuum and are not accessible by standard quantum-chemistry methods.
- Within non-Hermitian quantum mechanics, resonances become L^2-integrable, discrete states with complex energies (the real part describes resonance position and the imaginary part describes the resonance width); this enables calculation of resonances by standard quantum chemistry methods.
- Non-Hermitian extensions of quantum chemistry include 1) scaling all coordinates of the Hamiltonian with a complex factor exp(i*θ) (the complex-scaling method); 2) using complex basis functions; 3) augmenting the Hamiltonian by a local complex absorbing potential i*η*W(r).
- EOM-CC methods provide an excellent platform for treating resonances because they efficiently include correlation and tackle multiple electronic states of different character in a balanced fashion.
- Energies, properties, and nuclear gradients are available for several complex-valued EOM-CC methods.



(a) Stabilization of the the $2\Pi_g$ resonance of N_2^- with increasing CAP intensity from EOM-EA-CCSD calculations



(b) The potential energy curve for the $^2\Pi$ resonance of CuF^- from CAP-EOM-CCSD calculations

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