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Complex basis functions for molecular resonances: Methodology and applications ALEC WHITE, Univ of California - Berkeley, C. WILLIAM MCCURDY, Univ of California - Davis, MARTIN HEAD-GORDON, Univ of California - Berkeley — The computation of positions and widths of metastable electronic states is a challenge for molecular electronic structure theory because, in addition to the difficulty of the many-body problem, such states obey scattering boundary conditions. These resonances cannot be addressed with nave application of traditional bound state electronic structure theory. Non-Hermitian electronic structure methods employing complex basis functions is one way that we may rigorously treat resonances within the framework of traditional electronic structure theory. In this talk, I will discuss our recent work in this area including the methodological extension from single determinant SCF-based approaches to highly correlated levels of wavefunction-based theory such as equation of motion coupled cluster and many-body perturbation theory. These approaches provide a hierarchy of theoretical methods for the computation of positions and widths of molecular resonances. Within this framework, we may also examine properties of resonances including the dependence of these parameters on molecular geometry. Some applications of these methods to temporary anions and dianions will also be discussed.

Alec White
Univ of California - Berkeley

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