

A general formalism of Fock space multireference coupled cluster method for investigating electronic resonances in molecules.

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Abstract: Electron correlation and relaxation effects play a substantial role in the formation and decay of resonance states. We have formulated a complex absorbing potential (CAP) combined with Fock space multireference coupled cluster (FSMRCC) method for the correlated calculations of resonance energy and width [1, 2]. This can describe the dynamic and non-dynamic electron correlation efficiently in the ionized or electron attached states. Accurate resonance parameters are obtained by solving a small complex non-Hermitian eigenvalue problem. We note that both the dynamical and nondynamical correlation effects are extremely important in determining the resonance states near the internuclear distance at which the resonance becomes a bound state. The inclusion of correlation in this case drastically alters the internuclear distance at which the resonance anionic curve crosses with the neutral target curve. Our method, CAP-FSMRCC, is a state-of-the-art method that opens the possibility of routine *ab initio* studies of resonances exploiting the power of coupled-cluster techniques.

References

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