Fragment-Based Restricted-Active-Space Configuration Interaction with Second-order Correction Embedding for Periodic Hartree-Fock Wave Function

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We present an embedding method for restricted-active-space configuration interaction with second-order perturbative correction (RASCI-PT2)[1] embedded in the periodic Hartree-Fock (HF) wave function. The method allows us to calculate the electronic structure of localized feature for fragment in periodic systems. We first outline the implementation of embedding scheme employing Crystal17[2], Cryscor[3], and Q-Chem[4]. To evaluate our embedding method, we calculated the energy profile of single-bond dissociation of carbon-fluoride of fluorinated graphane, and the electronic excitation energies in covalent-organic framework. The results suggest that RASCI-PT2 embedded in HF wave function can be a promising tool for studying local properties of solid state.

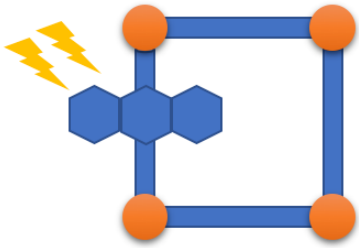

Figure 1: Example for a target system: a photoactive center in a periodic covalent-organic framework (COF).

References

1. Casanova, D. *J. Chem. Phys.* **2014**, *140*.
2. R. Dovesi, A. Erba, R. Orlando, C. M. Zicovich-Wilson, B. Civalleri, L. Maschio, M. Rerat, S. Casassa, J. Baima, S. Salustro, B. Kirtman. *WIREs Comput Mol Sci*. **2018,** *8*.
3. Pisani, C.; Schütz, M.; Casassa, S.; Usvyat, D.; Maschio, L.; Lorenz, M.; Erba, A. *Phys. Chem. Chem. Phys.* **2012**, *14*.
4. Shao, Y.; Gan, Z.; Epifanovsky, E.; Gilbert, A. T. B.; Wormit, M.; Kussmann, J.; Lange, A. W.; Behn, A.; Deng, J.; Feng, X.; et al. *Mol. Phys.* **2015**, *113*.