

Models of organometallic complexes for optoelectronic applications: from relativistic DFT to effective Hamiltonian models

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Organometallic complexes have potential applications as the optically active components of organic light emitting diodes (OLEDs) and organic photovoltaics (OPV). Development of more effective complexes may be aided by understanding their excited state properties. Here we discuss two key theoretical approaches to investigate these complexes: first principles atomistic models and effective Hamiltonian models. We discuss applications of these methods, such as, determining the nature of the emitting state, predicting the fraction of injected charges that form triplet excitations, and explaining the sensitivity of device performance to small changes in the molecular structure of the organometallic complexes [1]. We highlight the importance of relativistic effects in giving a accurate quantitative description of the optical properties of these materials (figure 1) [2] and the importance of effective Hamiltonians for understanding trends across materials and motivating design criteria [1].

Figure 1: Comparison of absorption (solid line) and magnetic circular dichroism (dashed line) spectra of fac-tris(1-methyl-5-phenyl-3-propyl-[1,2,4]triazolyl)iridium(III) to the excitation spectra calculated for this material from TDDFT. Three different calculations are shown: (a) non-relativistic, (b) scalar relativistic and (c) scalar relativistic with a spin-orbit perturbation. Both the scalar relativistic and spin-orbit effects are important to correctly predict the spectra of this, and other related, organometallic compounds.

References

[1] A. C. Jacko, B. J. Powell and R. H. McKenzie, [arXiv:1005.3897](https://arxiv.org/abs/1005.3897)

[2] A. R. G. Smith, M. J. Riley, S. C. Lo, P. L. Burn, I. R. Gentle and B. J. Powell, unpublished

