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Poster: Linear Response in Relativistic Dirac–Kohn–Sham Quantum-Electrodynamical Density Functional Theory

We derived and implemented relativistic QEDFT in linear response regime. The electrons are treated at the four-component Dirac–Kohn–Sham level of theory and coupled to transverse photons treated as dynamical variables. We show that light–matter coupling can enhance the strength of usually weak singlet–triplet transitions via a new type of spin–orbit interaction mediated by cavity photons.

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