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Singlet-Fission from First-Principles Many-Body Perturbation Theory[1] SIVAN REFAELY-ABRAMSON, Molecular Foundry, Lawrence Berkeley National Lab; Dept. of Physics, University of California Berkeley, CA, USA, FELIPE H. DA JORNADA, STEVEN G. LOUIE, Dept. of Physics, University of California Berkeley; Materials Sciences Division, Lawrence Berkeley National Lab, CA, USA, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Lab; Dept. of Physics, University of California Berkeley; Kavli NanoScience Institute, Berkeley, CA, USA — We present an ab initio approach to investigate the interaction between single excitons and non-interacting biexcitons from first-principles using many-body perturbation theory within the GW approximation and the Bethe-Salpeter Equation approach. We apply our model to explore singlet-fission in acene molecular crystals. For these systems, we calculate the electronic coupling between singlet excitations and non-interacting but spin-correlated triplet pairs, explore the resulting singlet-fission rate, and associate the exciton-exciton coupling mechanism in terms of the crystal structure and given the nature and symmetry of the involved solid-state excitons.

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Sivan Refaely-Abramson
Lawrence Berkeley National Lab; University of California Berkeley

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