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Effect of Crystal Packing on the Electronic Properties of Molecular Crystals

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Large scale quantum mechanical simulations are performed to study the effect of crystal packing on the electronic and optical properties of molecular crystals, which are essential for applications in organic electronics and photovoltaics. For structure prediction, we use the massively parallel genetic algorithm (GA) package, GAtor, which relies on the evolutionary principle of survival of the fittest to find low-energy crystal structures of a given molecule. Dispersion-inclusive DFT, implemented in the FHI-aims code, is used for structural relaxation and energy evaluations. The structure generation package, Genarris, performs fast screening of randomly generated structures with a Harris approximation, whereby the molecular crystal density is constructed by replicating the single molecule density, which is calculated only once. Many-body perturbation theory, within the GW approximation and the Bethe-Salpeter equation (BSE), as implemented in the BerkeleyGW code, is employed to describe properties derived from charged and neutral excitations. We show that transport, optical absorption, and singlet fission efficiency may be enhanced by modifying the crystal packing of TCS3 and rubrene.