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**High-throughput organic semiconductor discovery combining tight-binding and first-principles calculations** ANDRE LEITAO BOTELHO, TIM MUELLER, Johns Hopkins University — We present the combination of a tight-binding model and first-principles calculations as a two-step screening for the accelerated discovery of organic semiconductors. For the tight-binding model, we select the adapted Su-Schrieffer-Heeger Hamiltonian for its ability to provide both the electronic structure and optimized geometry based solely on the structural formula. We produce two sets of parameters, one to match the optical gaps to exciton energies from TDDFT, and another set to match the transport gaps to HOMO/LUMO energies from DFT with an experimental correction factor. Although the fittings use fewer than one thousand oligomers, the predictive results for the remaining one million oligomers agree with DFT (coefficient of determination of up to 0.8) and can be used as a pre-screening step. With the same set of parameters, we also calculate the charged states to predict the Marcus theory reorganizational energies as an estimate the conductivities of holes and electrons. Based on the calculated properties, we discuss materials selection for photovoltaics and transistors.

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