

Abstract Submitted
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Massive computational search for n-type organic semiconductors¹

ANDRE LEITAO BOTELHO, TIM MUELLER, Department of Materials Science and Engineering, Johns Hopkins University — In a search for n-type organic materials, which are rare compared to p-type, we calculate the optimized geometries and electronic structures for millions of conjugated oligomers. A good n-type material (electron conductor) must have a low-lying LUMO level (high electron affinity) in order to avoid chemical reactions that create electron traps. For high conductivity, it must have a low barrier to electron hopping, indicated by an internal reorganization energy in the meV range. The calculations use the adapted Su-Schrieffer-Heeger tight-binding Hamiltonian and include both neutral and singly charged structures. The group of structures with a combination of low-lying LUMO levels and small internal reorganization energies is presented as candidates for n-type organic semiconductor materials. The data are also used to directly compute the optical band gaps and exciton binding energies, while the HOMO and LUMO levels are used to estimate cyclic voltammetry oxidation and reduction potentials. Application of the methodology to other organic materials searches is discussed.

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