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Charge patching method for the calculation of electronic structure of organic semiconductors[1] NENAD VUKMIROVIC, LIN-WANG WANG, Lawrence Berkeley National Laboratory — The electronic structure of organic semiconducting conjugated polymers and molecular crystals is essential in determining their optical and transport properties. Such organic semiconductor systems have potential applications for solar cells, field-effect transistors and luminescent devices. However, for such systems containing a large number of atoms, the direct calculations based on density functional theory (DFT) are often not feasible. Here, we present the development of the charge patching method for the calculations of organic systems, a method which was previously successful in treating inorganic semiconductor materials [1]. The results of the calculations for alkane and alkene chains using this approach yield the difference in Kohn-Sham wavefunction eigen energies of the order of only 30 meV compared with direct DFT calculations. Further investigations involving aromatic compounds, as well as elements such as sulfur, nitrogen, and oxygen, will be presented. [1] L.W. Wang, Phys. Rev. Lett. 88, 256402 (2002).

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