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Site energies and charge transfer rates near pentacene grain boundaries from first-principles calculations HAJIME KOBAYASHI, YUICHI TOKITA, Sony Co. — Charge transfer rates near pentacene grain boundaries are derived by calculating the site energies and transfer integrals of 37 pentacene molecules using first-principles calculations. The site energies decrease considerably near the grain boundaries, and electron traps of up to 300 meV and hole barriers of up to 400 meV are generated. The charge transfer rates across the grain boundaries are found to be reduced by three to five orders of magnitude with a grain boundary gap of 4 Å because of the reduction in the transfer integrals. The electron traps and hole barriers also reduce the electron and hole transfer rates by factors of up to 10 and 50, respectively. It is essential to take the site energies into consideration to determine charge transport near the grain boundaries. We show that the complex site energy distributions near the grain boundaries can be represented by an equivalent site energy difference, which is a constant for any charge transfer pass. When equivalent site energy differences are obtained for various grain boundary structures by first-principles calculations, the effects of the grain boundaries on the charge transfer rates are introduced exactly into charge transport simulations, such as the kinetic Monte Carlo method.

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