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First-
Principle Study of the Charge Transport in PTCDA/Ag(111) Interfaces
TATSUHIKO OHTO, HISAO NAKAMURA, KOICH YAMASHITA, Department of Engineering, The University of Tokyo — We focused on the transport property of organic / metal interfaces, which is one of the central issues in organic based devices as well as the prototype of charge injection at interface. We performed first principle calculations for the interface between 3, 4, 9, 10 – perylenetetracarboxylic dianhydride (PTCDA) molecules and Ag (111) surface based on non-equilibrium Green's function method combined with the density functional theory. In the present report, the range of the coverage of PTCDA was taken from a single molecule region (< 1 ML) to 3 ML. We found hybrid interfacial states between the large aromatic part of PTCDA and Ag (111) substrate, and they have characteristic effective masses along the stacking direction of PTCDA molecules. Energy level alignments and effective masses relating to these hybrid interfacial states are quite sensitive to the coverage. We will report detail transport properties such as transmission coefficients and show the comparison with the properties of molecular crystals of PTCDA.

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