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Theoretical study on the surface complex between TiO2 and hetero-TCNQ YUHEI SHIMODA, RYOTA JONO, Department of Chemical System Engineering, School of Engineering, The University of Tokyo, HIROSHI SEGAWA, Research Center for Advanced Science and Technology, The University of Tokyo, KOICHI YAMASHITA, Department of Chemical System Engineering, School of Engineering, The University of Tokyo — Interfacial charge transfer transitions between organic and inorganic materials are expected to be a potential photoinduced charge separation mechanism for photoenergy conversions. Recently, we have reported that the hybrid material formed from TiO_2 nanoparticles and an organic electron acceptor, 7,7,8,8-tetracyanoquinodimethane (TCNQ), shows strong interfacial charge transfer absorption in the visible region [1-3]. In the present work, we have investigated the molecular and optical properties of the surface complexes of TiO_2 and hetero-TCNQ: furan-TCNQ, thiophene-TCNQ, and selenophene-TCNQ, which are considered to promote light absorption in the near-IR region more efficiently than TiO_2-TCNQ. The redox potentials of these hetero-TCNQ are calculated to be lower than that of TCNQ. We calculated these hetero-TCNQ and the surface complexes between those and a TiO_2 nano cluster, using the density functional theory (DFT) and time-dependent DFT methods. [1] R. Jono, J. Fujisawa, H. Segawa, and K. Yamashita, J. Phys. Chem. Lett., 2, 1167-1170 (2011). [2] S. Manzhos, R. Jono, K. Yamashita, J. Fujisawa, M. Nagata, and H. Segawa, J. Phys. Chem. C, 115, 21487-21493 (2011). [3] R. Jono, J. Fujisawa, H. Segawa, and K. Yamashita, Phys. Chem. Chem. Phys., 15, 18584-18588 (2013).

Yuhei Shimoda
Tokyo University

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