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First-principles study of atomic and electronic structures of coumarin dyes adsorbed on titania surface HIROYOSHI MOMIDA, Institute of Industrial Science, University of Tokyo, TAKAHISA OHNO, CMSC, National Institute for Materials Science and Institute of Industrial Science, University of Tokyo — The coumarin dyes are good photo-sensitizers for the dye-sensitized solar cell due to the wide absorption energy range of the visible light and the fast photo-induced charge injection from the dyes to the titania. The dyes are adsorbed on the Ti sites via the carboxyl group, but detailed adsorbed structures and effect on the electronic structures are unknown. We performed the first-principles calculations of the coumarin343 and NKX2311 dyes adsorbed on the rutile titania (110) for three types of the contact structures. We found that the bidentate type is energetically more stable than the ester-like and molecular types. The HOMO-LUMO gap of the NKX2311 is smaller than that of the coumarin343, consistent with the experiments. This work was partly supported by the RISS project in IT program and a Grant-in-Aid for Scientific Research (No.17064017) of MEXT of the Japanese Government.

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