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First-principles study on Ru(4,4',4"-tricarboxy-2,2':6',2"-terpyridine)$(NCS)_3$ sensitizer on TiO_2 anatase(101) surface: Adsorbed structures and electronic states for dye-sensitized solar cells[1] KEITARO SODEYAMA, MASATO SUMITA, YOSHITAKA TATEYAMA, National Institute for Materials Science MANA — Dye-sensitized solar cells are expected as a cost effective solar-to-electricity energy conversion devices. The efficiency of the power conversion is greater than 10% when Ru(II) polypyridyl sensitizers are used. For further improvement of the efficiency, we need to understand the adsorbed structures at atomistic level in detail. In this study, we investigated the adsorbed structures of Ru(4,4',4"-tricarboxy-2,2':6',2"-terpyridine)$(NCS)_3$ sensitizer on TiO_2 anatase(101) surface. For four possible adsorbed structures (two candidates have one adsorbed carboxyl group(one-leg) and the others have two adsorbed groups(two-leg)), we found the adsorption energies are quite similar within 0.4 eV. This is attributed to the presence of the hydrogen bond between the hydrogen of carboxyl group and the oxygen of the surface in the one-leg structure. We also calculated the excited states of the four structures of the sensitizer by TDDFT and found that the UV spectrum shift depending on the structure differences.

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