ELECTRONIC SUPPORTING INFORMATION

Structure and energy level alignment at dye-electrode interface in p-type DSSC: new hints on the role of anchoring modes from *ab initio* calculations.

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Figure S1. Atom- and angular-momentum projected density of states (PDOS) of (a) pristine NiO(100) slab and (b) p-type NiO(100) slab at the DFT+U level of theory with $(U\text{-}J)_{Ni}$=3.8 eV. Ni d (black line) and O p (red line) states are shown; the Fermi energy (E_F) is set to zero. (c) NiO(100) five-atomic-layer slab model, the highlighted Ni atom (in yellow) is removed for modeling p-type NiO(100); color legend: Ni (grey) O (red).

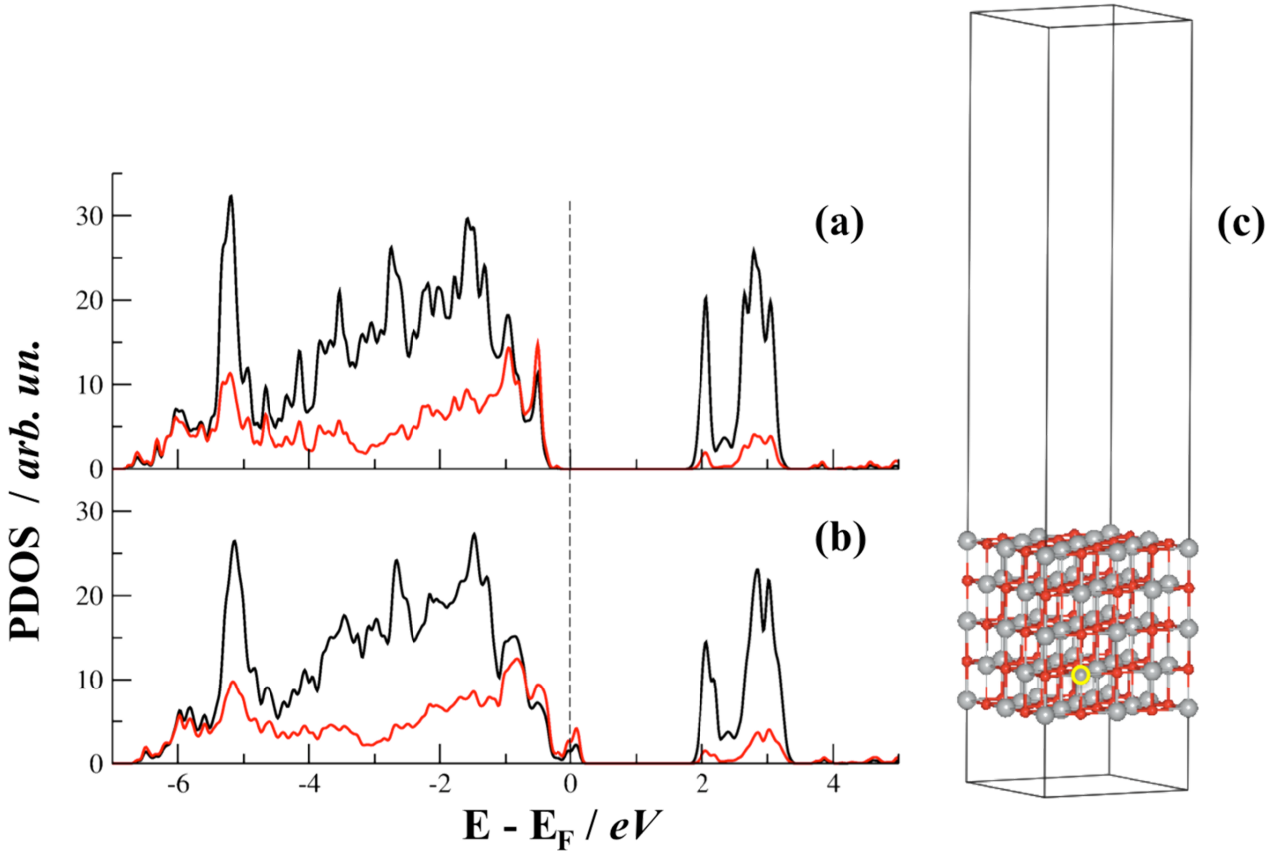

Figure S2. Plane-averaged electrostatic potential energy (solid line) along the *z* direction (i.e. the perpendicular axis to the slab surface) for the clean p-type NiO slab (a), p-NiO/CCO_2-M (b), p-NiO/CCO_2-B (c), p-NiO/CPO_3-M (d), p-NiO/CPO_3-B (e) p-NiO/CPO_3-T (f); dashed lines represent the corresponding Fermi energy (i.e., the highest occupied Kohn-Sham eigenvalue).