Supplementary Information for

N-promoted Ru_{1}/TiO_{2} single-atom catalysts for photocatalytic water splitting for hydrogen production: A density functional theory study

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The periodically repeated slabs consisting of four atomic layers, separated by a vacuum region of 15 Å, are adopted to mimic the (111) surfaces of Pt, Pd, and Ni. A 2 x 2 surface cell and Monkhorst-Pack k-point mesh of 3 x 3 x 1 are used for all calculations. The bottom two layers are fixed at the optimized bulk lattice constants, and the top two layers and the adsorbate (i.e., the H atom) are fully relaxed. The H atom is in the fcc site, rather than other sites (Figure S1). The dipole correction is taken into account in all cases.

Figure S1  Atomic structures of pure (left) and H-adsorbed (right) Ni (111) surfaces under our investigation (top view). The big blue and small white balls denote the Ni and H atoms, respectively.