Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A novel design of SiH/CeO_2(111) van der Waals type-II heterojunction for water splitting

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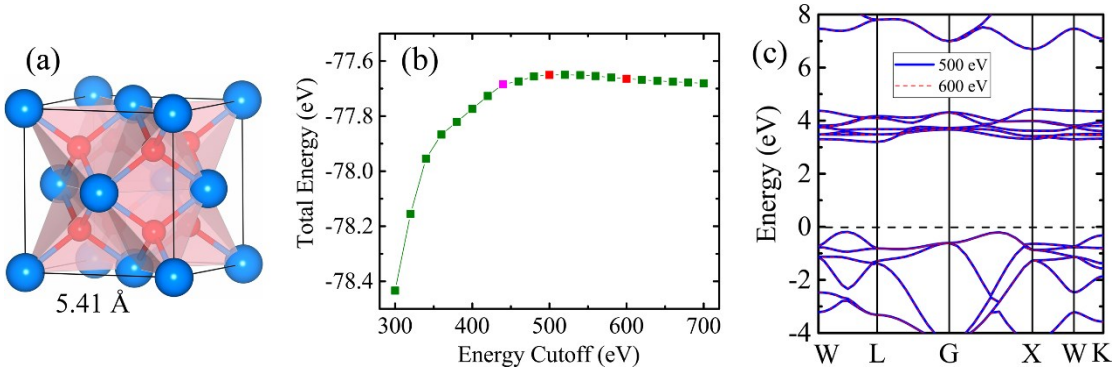

Figure S1. (a) CeO_2 in a fluorite structure. (b) Total energy of CeO_2 calculated with different energy cutoff. (c) Band structure of CeO_2 calculated with energy cutoff of 500 eV and 600 eV. Clearly, the calculated total energy of CeO_2 tends to be stable when the energy cutoff is greater than 425 eV, so it is reasonable to set the energy cutoff to be greater than 425 eV. In this study, the energy cutoff is set to 500 eV. There is no difference in the band structure of CeO_2 calculated with energy cutoff of 500 eV and 600 eV, which further proves that the energy cutoff selected in this study is reasonable.

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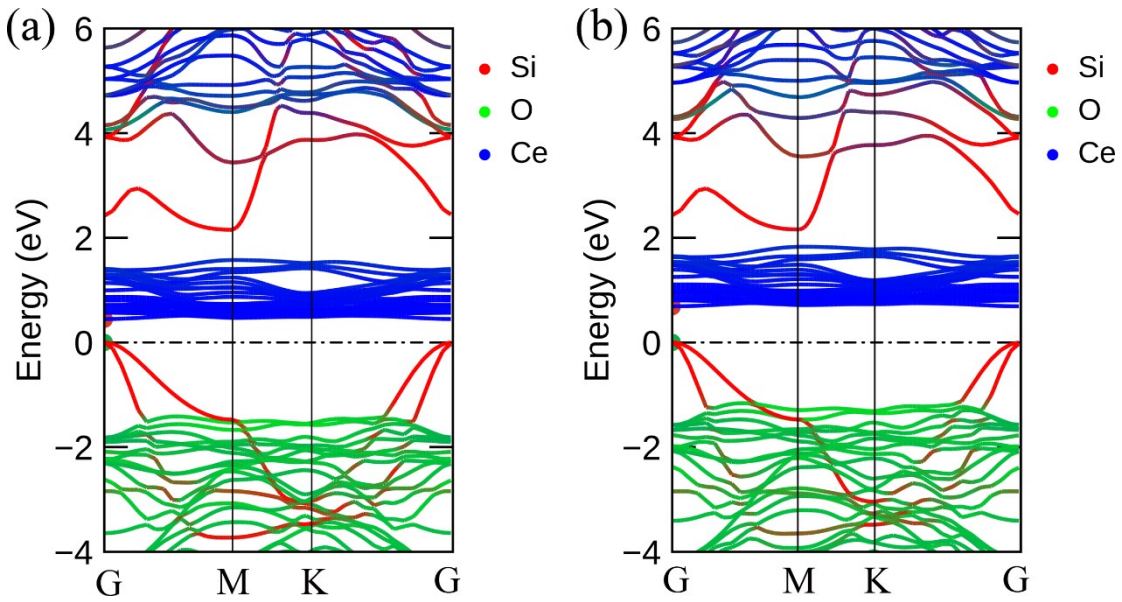

Figure S2. PBE results of the projected band structure of the (a) first and (b) second stacking modes in Figure 2. Although the adhesive energies of different stacking models are different, the effect on their electronic structures is almost negligible.

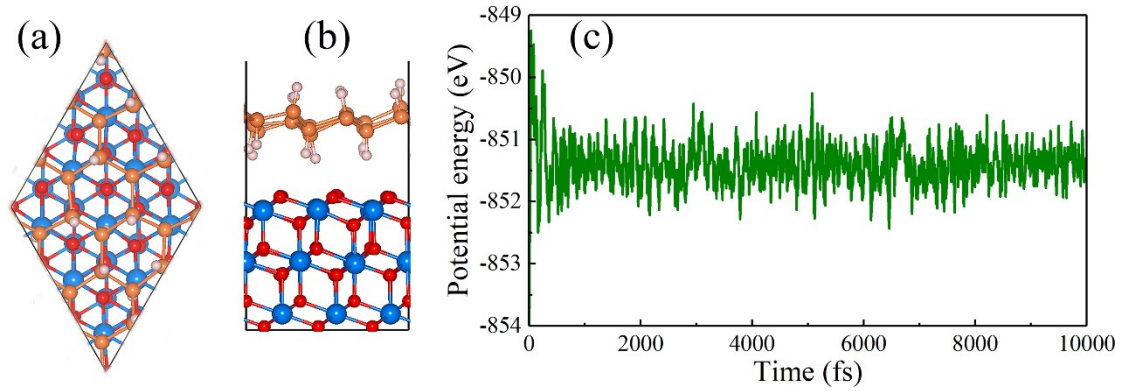

Figure S3. (a) Top and (b) side views of the snapshot from the molecular dynamics simulation of atomic structures for the 3×3 SiH/CeO_2(111) heterojunction at 300 K. (c) Variation of the total potential energy in the molecular dynamics simulation at room temperature during the time scale of 10.0 ps.

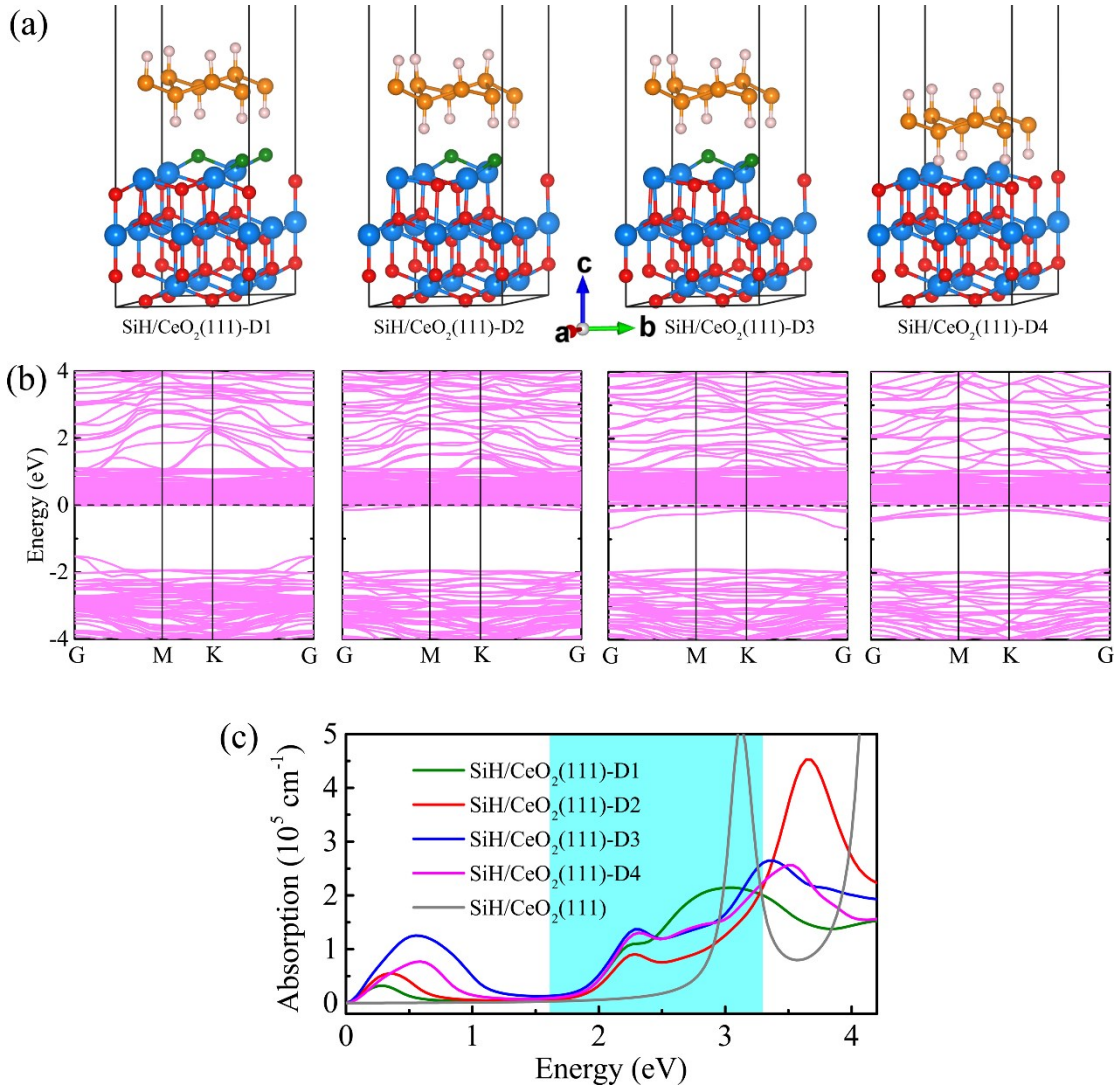

Figure S4. (a) The geometric structures of SiH/CeO_2(111) with one, two, three, and four oxygen vacancies on the surface, denoted as SiH/CeO_2(111)-D1, SiH/CeO_2(111)-D2, SiH/CeO_2(111)-D3, and SiH/CeO_2(111)-D4, respectively. The oxygen atoms on CeO_2(111) surface are highlighted by green spheres. (b) Band structures of SiH/CeO_2(111)-D1, SiH/CeO_2(111)-D2, SiH/CeO_2(111)-D3, and SiH/CeO_2(111)-D4. (c) Optical absorption spectra of SiH/CeO_2(111)-D1, SiH/CeO_2(111)-D2, SiH/CeO_2(111)-D3, SiH/CeO_2(111)-D4, and SiH/CeO_2(111).