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

Supplementary Material: The effects of c-Si/a-SiO_2 interface atomic structure on its band alignment: an *ab initio* study

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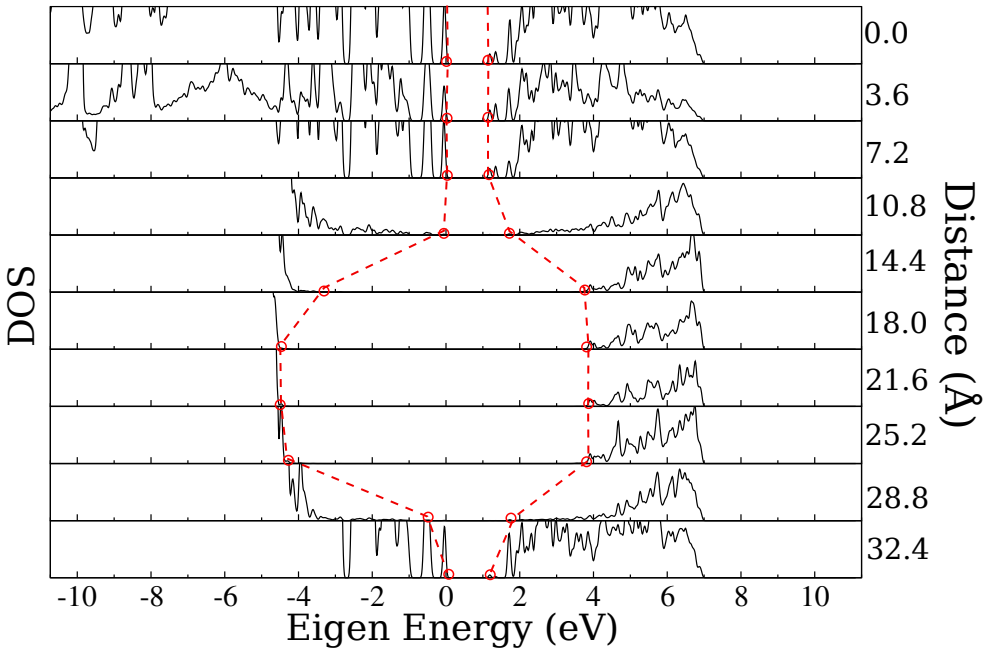

FIG. S1. The selected density of states (DOS) summed for the atoms within a distance range along the [001] direction for HSE calculated n=**2** structure. From top to bottom, it follows from Si-part to SiO_2-part. The distance on the right side corresponds to the x-axis of Fig.5 and 6 in the main text. Red circles indicate the band edge positions.

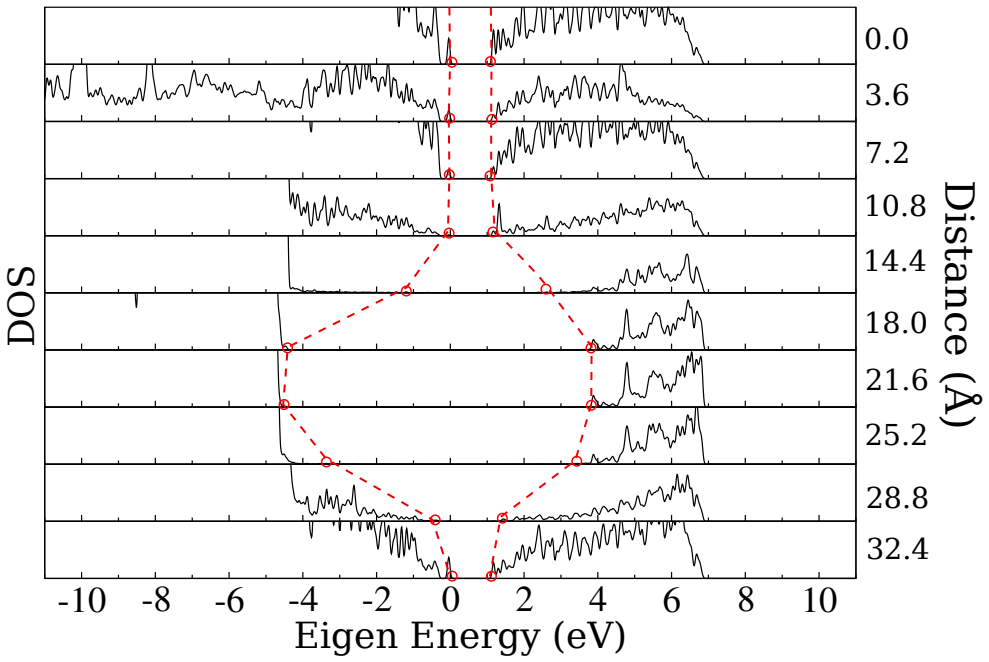

FIG. S2. The selected density of states (DOS) summed for the atoms within a distance range along the [001] direction for HSE calculated n=**3** structure. From top to bottom, it follows from Si-part to SiO_2-part. The distance on the right side corresponds to the x-axis of Fig.5 and 6 in the main text. Red circles indicate the band edge positions.

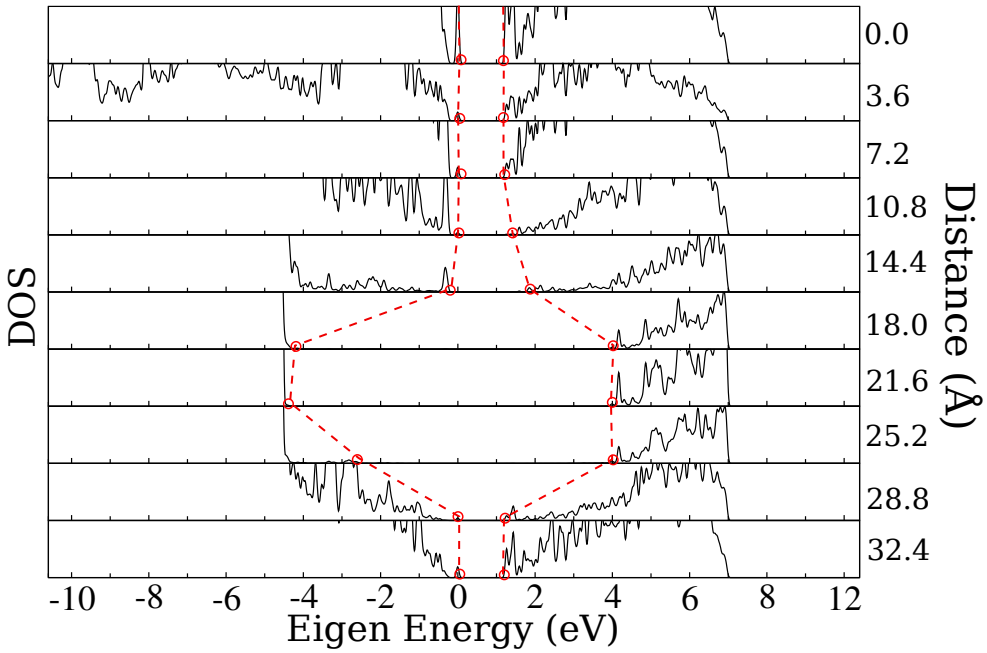

FIG. S3. The selected density of states (DOS) summed for the atoms within a distance range along the [001] direction for HSE calculated n=**4** structure. From top to bottom, it follows from Si-part to SiO_2-part. The distance on the right side corresponds to the x-axis of Fig.5 and 6 in the main text. Red circles indicate the band edge positions.