Supporting Information

Oxygen Vacancy as Active Site for H_2S Dissociation on Rutile TiO_2 (110) Surface: A First-principles Study

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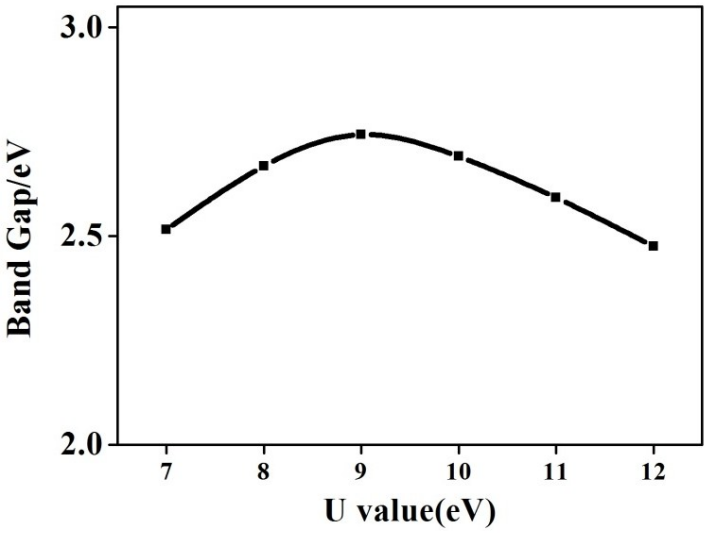

Fig. S1 Variation of band gaps with different U parameters for rutile TiO_2.

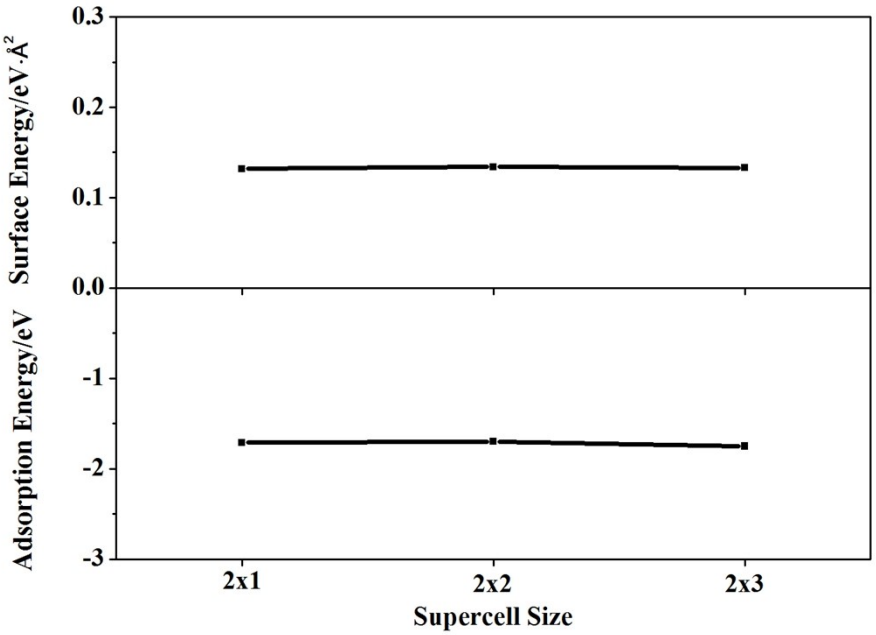

Fig. S2 Convergence tests of Surface energies and H_2S adsorption energies for the perfect surface, respectively.

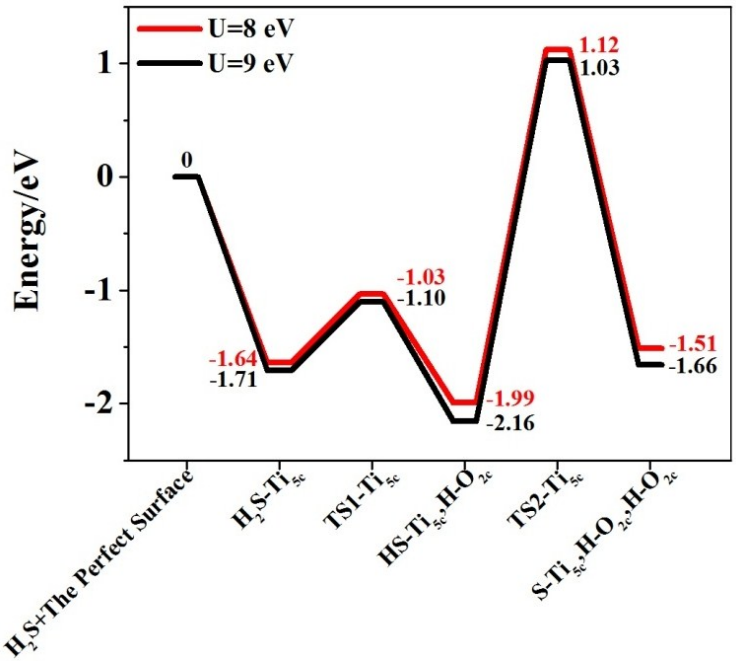

Fig. S3 Energy profiles for the dissociation of H_2S on the perfect surface calculated by different U parameters.

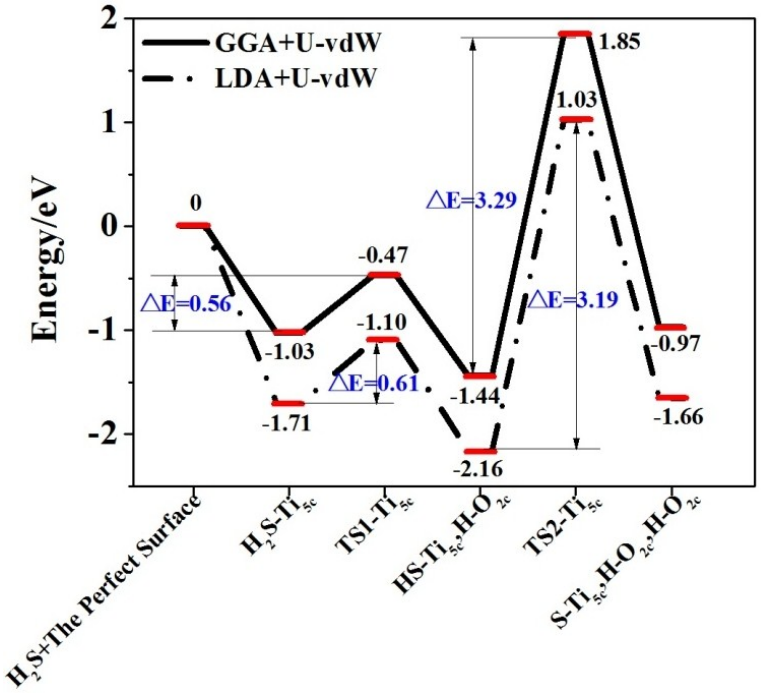

Fig. S4 Energy profiles for the H_2S dissociation on the perfect surface from dispersion corrected GGA+U and LDA+U, respectively.

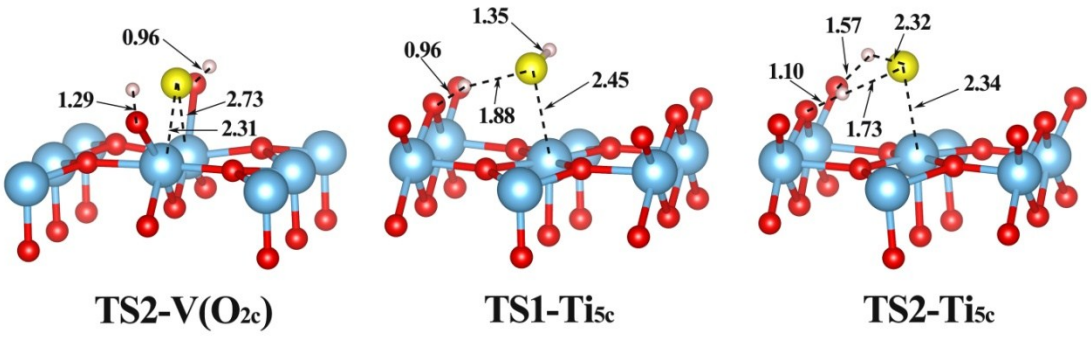

Fig. S5 Configurations of transition states. The bond length is in Å.

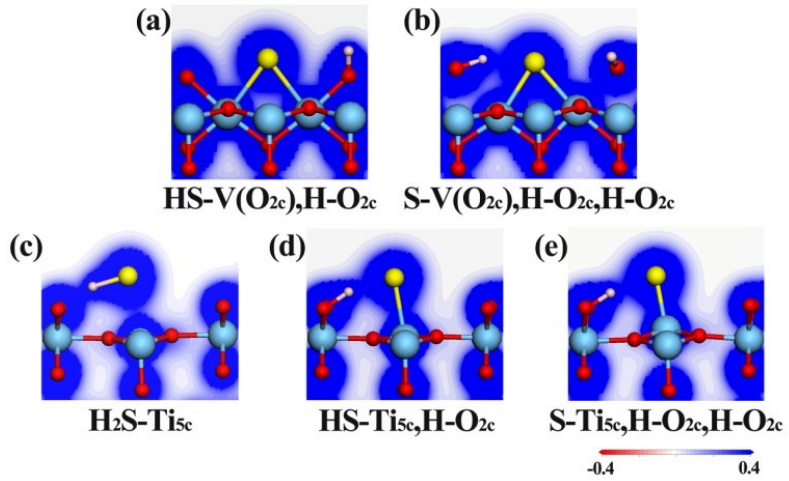

Fig. S6 The total electron densities of HS/H (a) and S/H/H (b) on the defected surface, and H_2S (c), HS/H (d) and S/H/H (e) on the perfect surface, respectively. The electron density is in electrons/Å^3.