Supporting Information

Identifying the role of excess electrons and holes for initiating photocatalytic dissociation of methanol on a TiO_2(110) surface

Ziyu Hu* and Fengdu Yu

College of Mathematics and Physics, Beijing University of Chemical Technology, Beijing, 100029, People's Republic of China. E-mail: huziyu@mail.buct.edu.cn

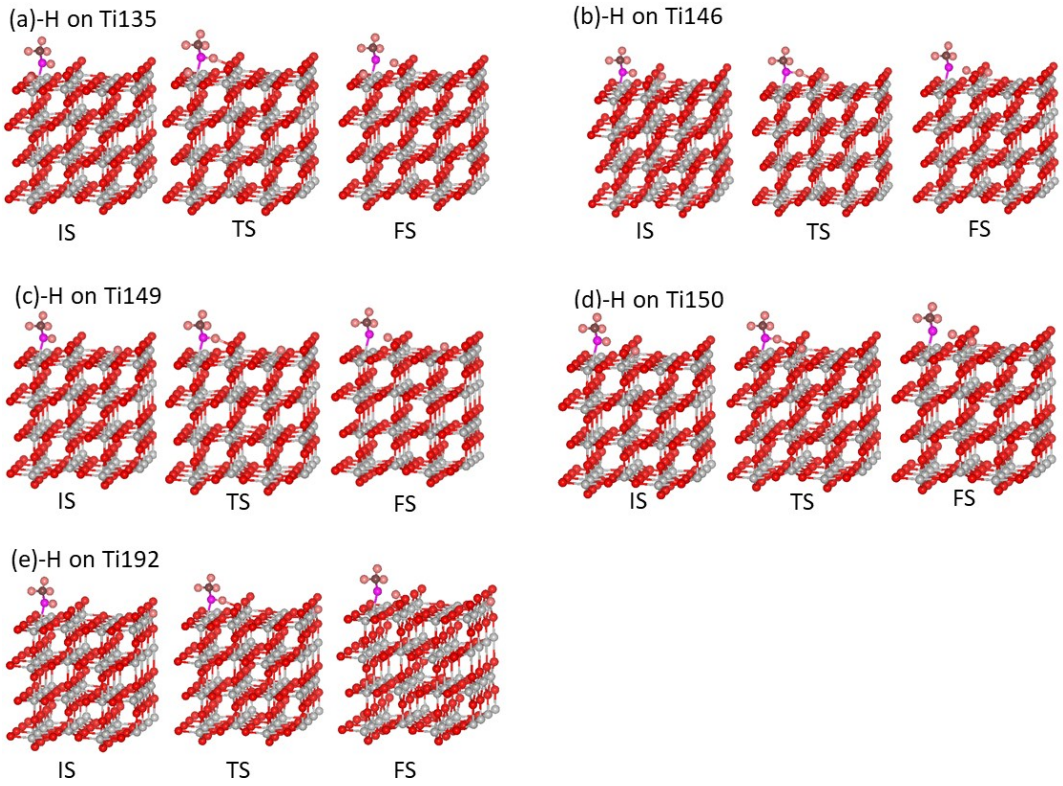

Fig. S1. The lateral structures for three adsorption states of the initial state (IS), transition state (TS) and final state (FS) for the different electrons introduced sites to methanol dissociation on TiO_2(110) are presented in (a-e). The grey, brown, pink and red balls are indicated titanium, carbon, hydrogen and oxygen atoms, respectively.

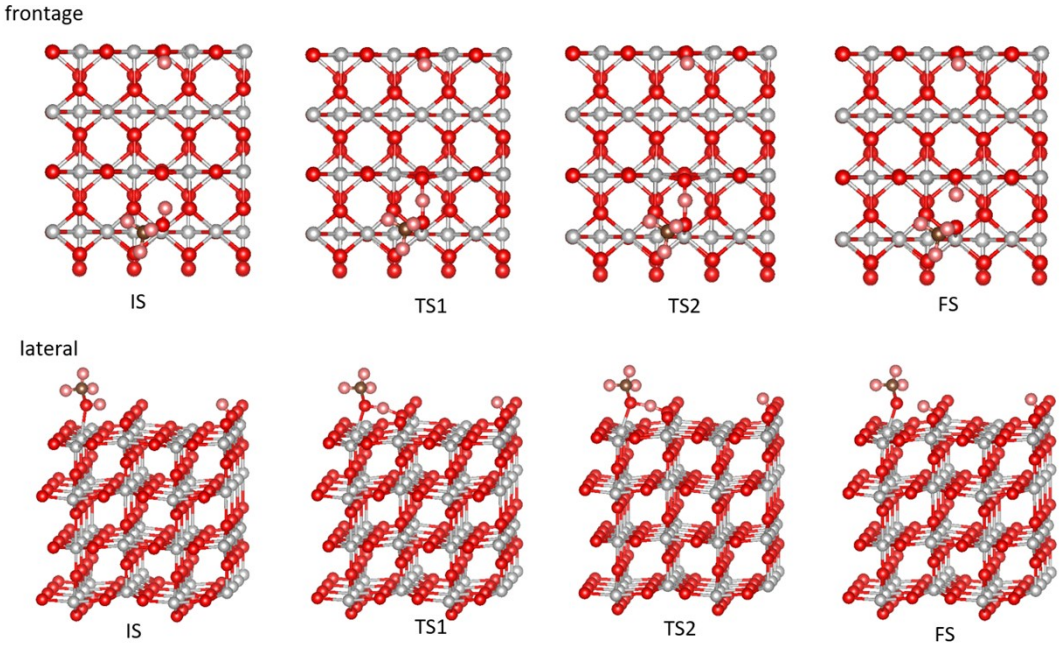

Fig. S2. The frontage and lateral structures for four adsorption states of the initial state (IS), transition state (TS1, TS2) and final state (FS) for the different electrons introduced sites on the subsurface TiO_2(110) are presented in (a-b). The grey, brown, pink and red balls are indicated titanium, carbon, hydrogen and oxygen atoms, respectively.