Supplementary Materials

Exploration of the active sites on the Rh-In_2O_3 catalyst for the semi-hydrogenation of acetylene: A theoretical study

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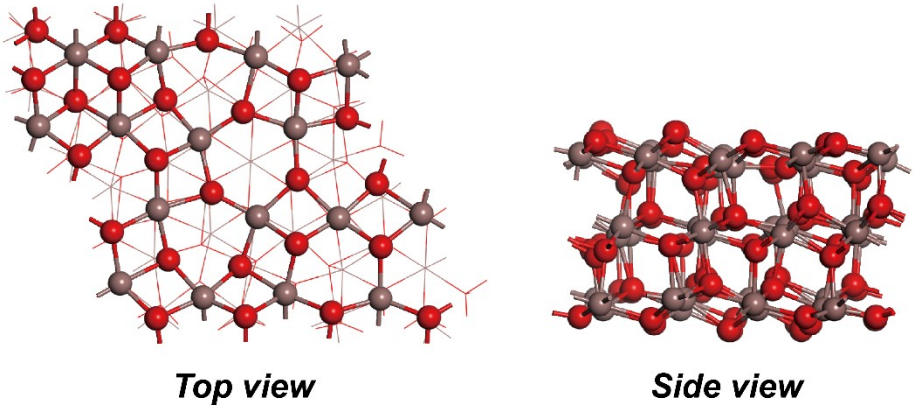

Fig. S1 Configuration of In_2O_3(111) model

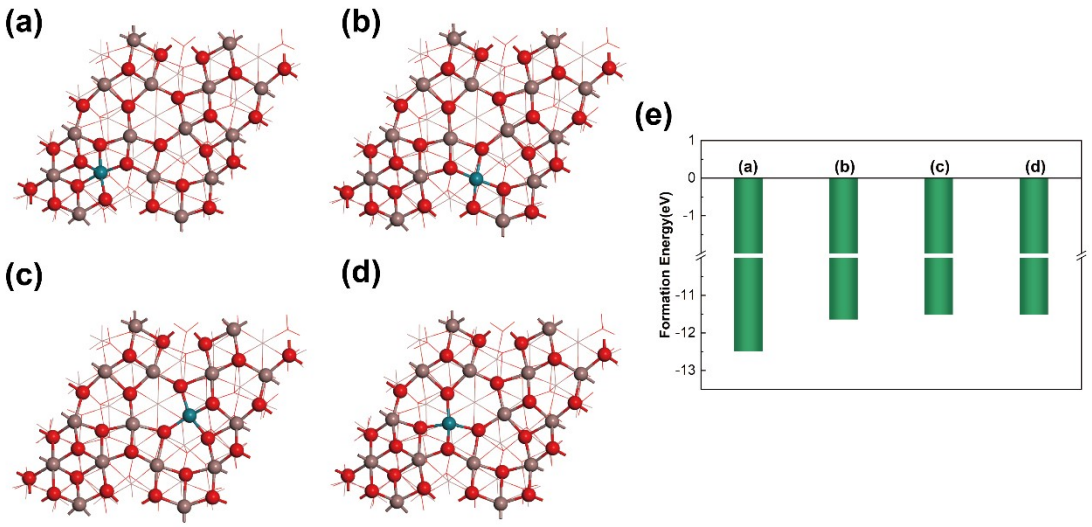

Fig. S2 Configurations of (a-d) four potential sites of Rh single atom and (e) the comparison of surface formation energies

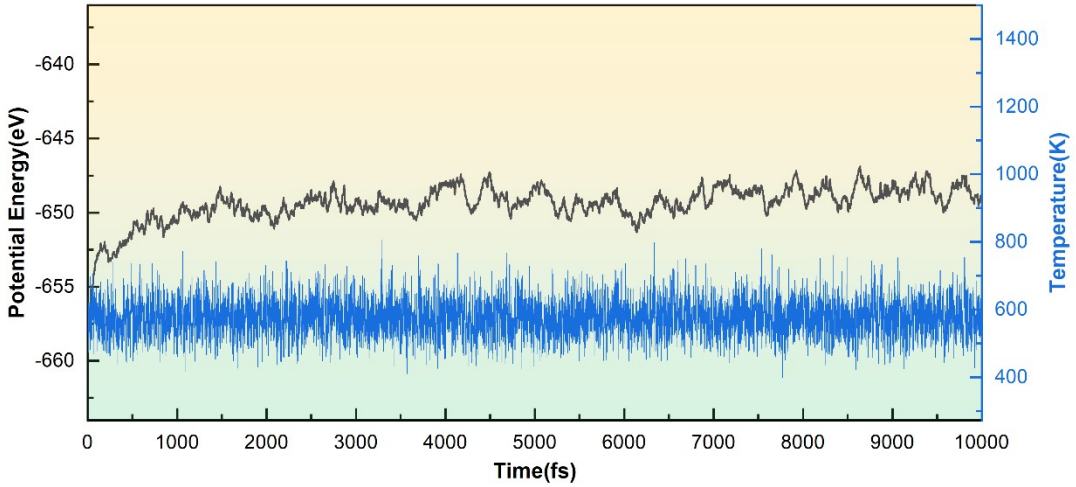

Fig. S3 The potential energy and temperature of the Rh_1/In_2O_3 model during the AIMD simulation

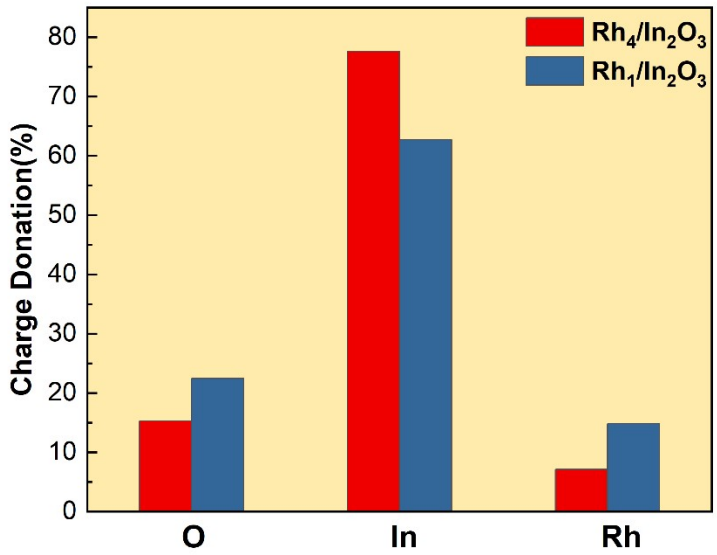

Fig. S4 The charge donation of oxygen vacancy over the Rh_4/In_2O_3 and Rh_1/In_2O_3 models

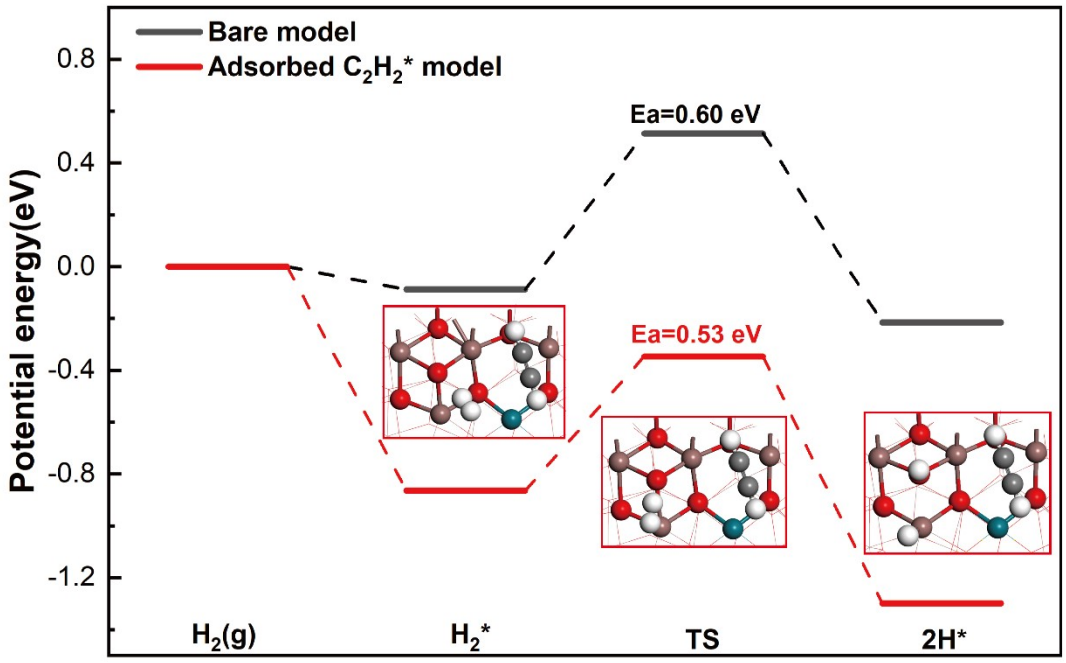

Fig. S5 Adsorption and dissociation of H_2 molecule over the Rh_1/In_2O_3_Ov site with and without C_2H_2 adsorption

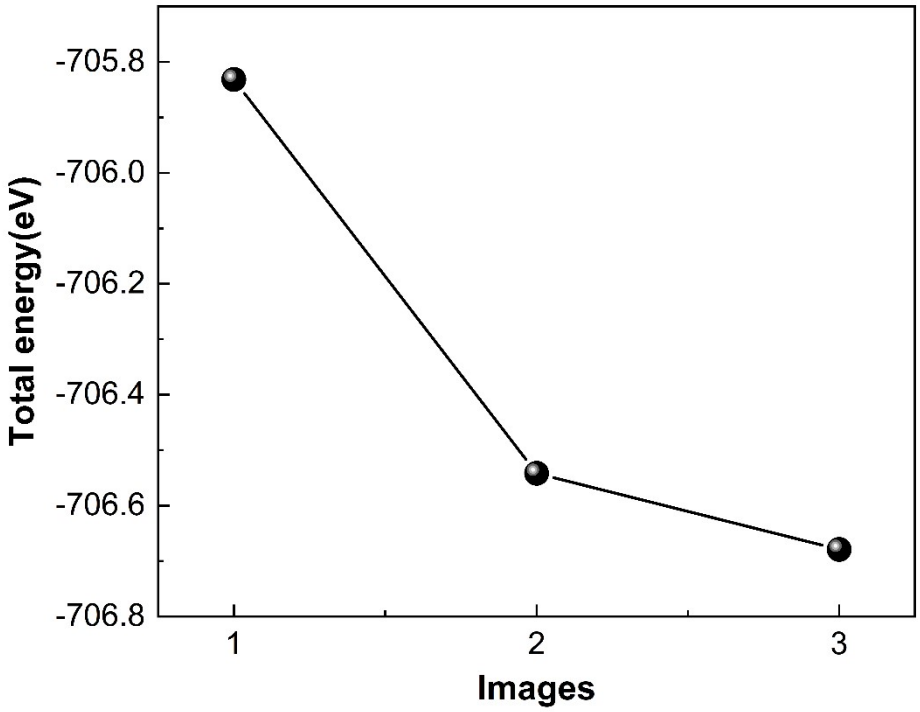

Fig. S6 CI-NEB trajectories for C_2H_2* hydrogenation to C_2H_3* over the supported Rh_4 site

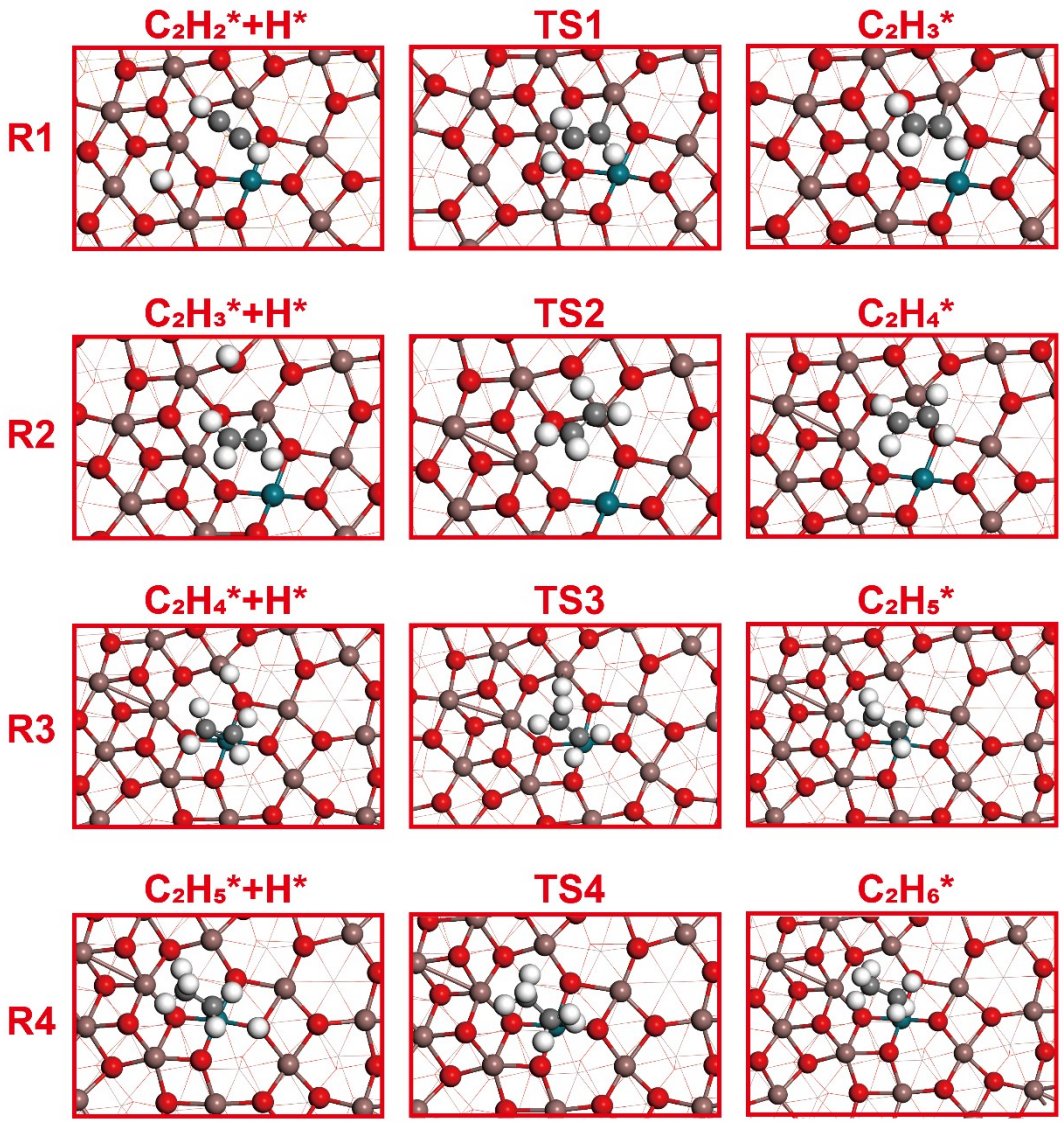

Fig. S7 Configurations of the intermediates involved acetylene hydrogenation over the Rh_1/In_2O_3_Ov site

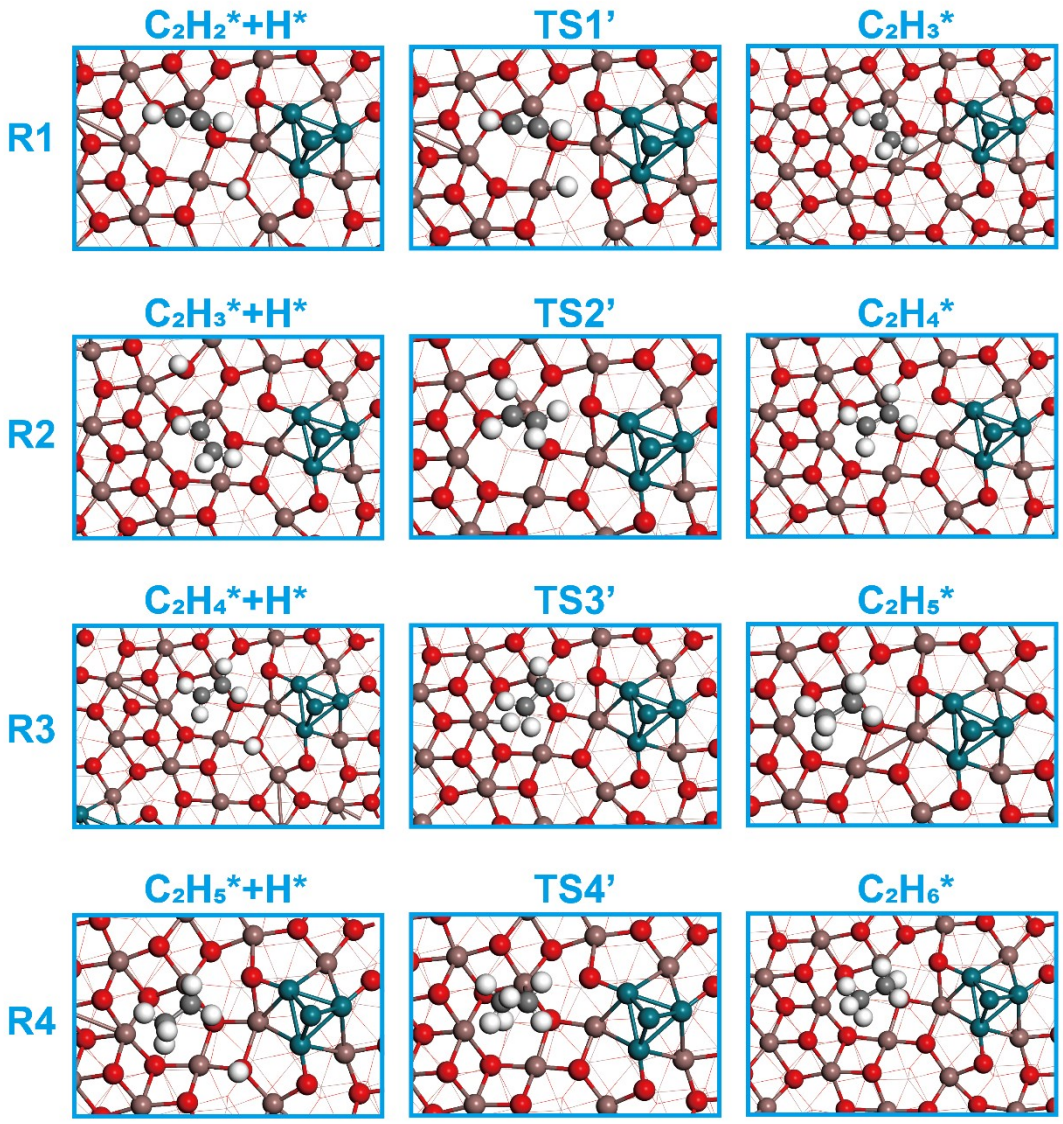

Fig. S8 Configurations of the intermediates involved acetylene hydrogenation over the Rh_4/In_2O_3_Ov site

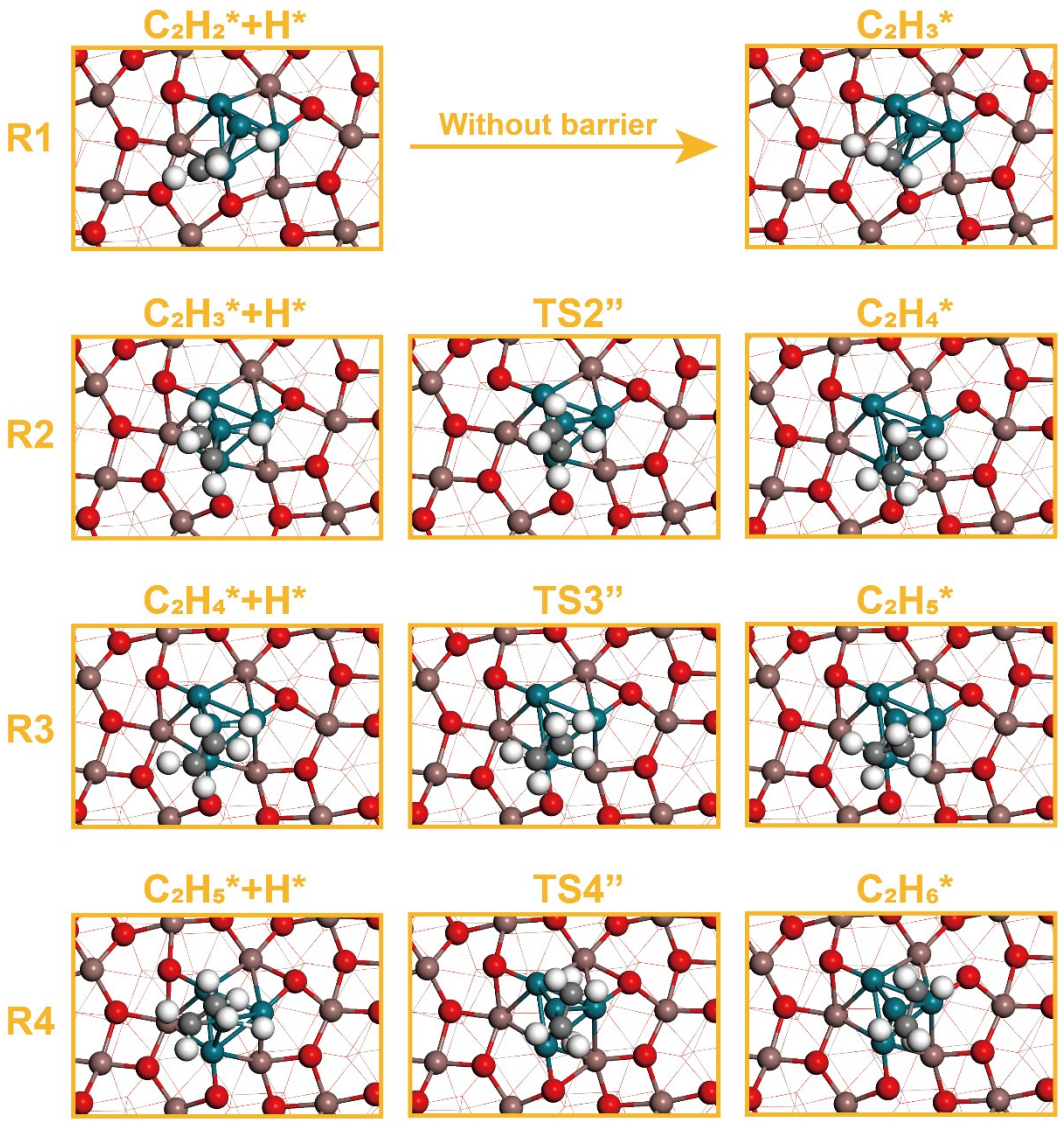

Fig. S9 Configurations of the intermediates involved acetylene hydrogenation over the $Rh_4/In_2O_3\_Rh_4$ site