Electronic Supplementary Material (ESI) for Catalysis Science & Technology.


# Electronic Supplementary Information

## Selective Hydrogenation of Acetylene over Cu(211), Ag(211) and Au(211): Horiuti-Polanyi Mechanism *vs*. Non-Horiuti-Polanyi Mechanism

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**Table S1** Adsorption/binding energies (eV) of $C_2H_2$, $C_2H_3$ and $C_2H_4$ on the possible adsorption sites over Cu(211), Ag(211) and Au(211). The corresponding input structures over Ag(211) are shown in Figure S1 as examples.

| | | Cu(211) | Ag(211) | Au(211) |
|---|---|---|---|---|
| $C_2H_2$ | B5 | -1.04 | 0.10 | -0.46 |
| | hcp | -1.36 | 0.06 | -0.56 |
| | fcc | -1.36[a] | 0.22 | -0.30 |
| $C_2H_3$ | bridge | -2.44 | -1.74 | -2.00 |
| | hcp | -2.44[a] | -1.74[a] | -2.00[a] |
| $C_2H_4$ | 2σ | -0.42 | -0.10 | -0.24 |
| | π | -0.54 | -0.21 | -0.35 |

[a] These structures changed to the most stable one after optimization.

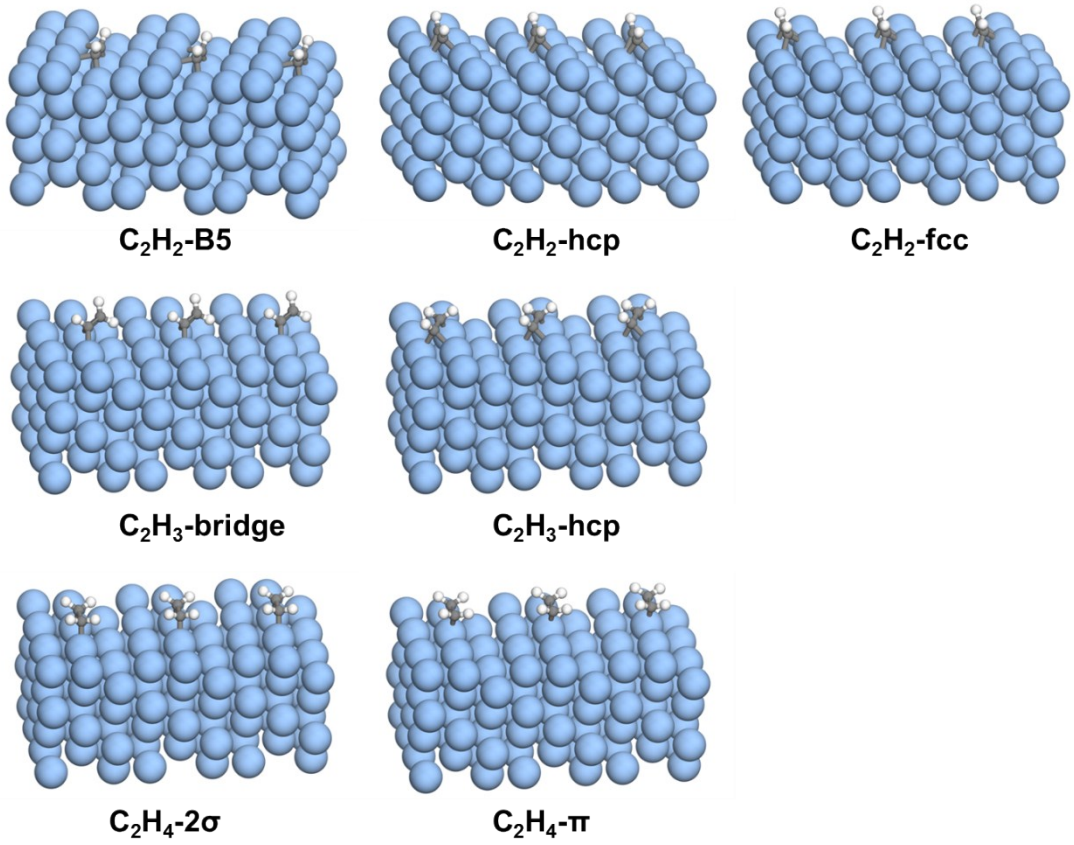


**Figure S1** Input structures of possible $C_2H_2$, $C_2H_3$ and $C_2H_4$ adsorption configurations.

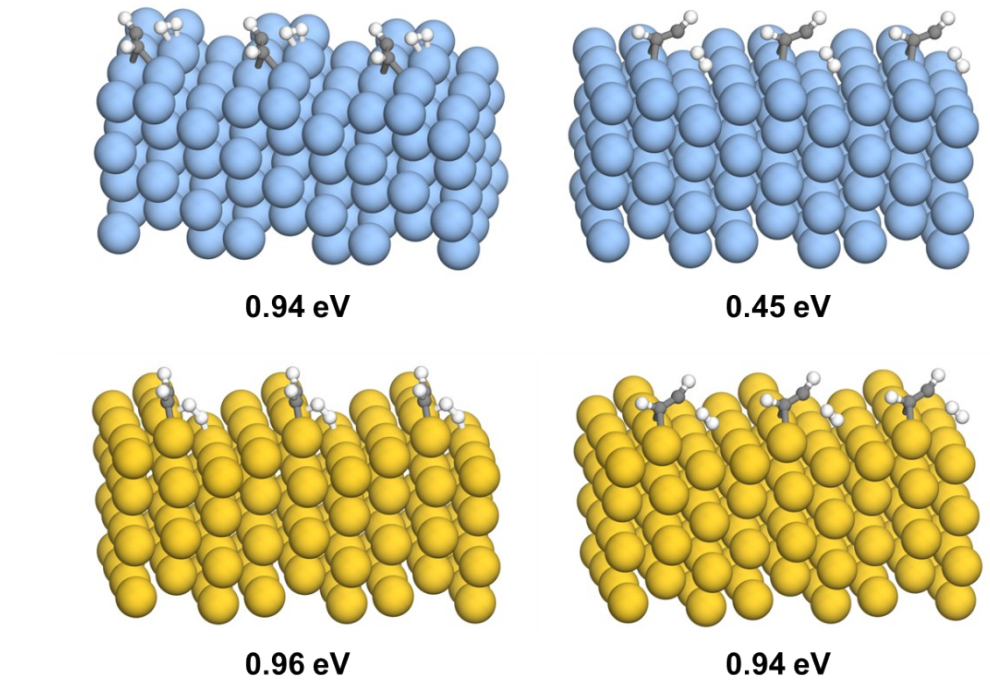


**Figure S2** Possible transition state structures of $C_2H_2$ hydrogenation with $H_2$ over Ag(211) and Au(211). The corresponding reaction barriers are also shown here.