Supplementary Materials for

CO_2 Activation and Dissociation on In_2O_3 (110) Supported PdnPt(4-n) (n = 0-4) Catalysts: A Density Functional Theory Study

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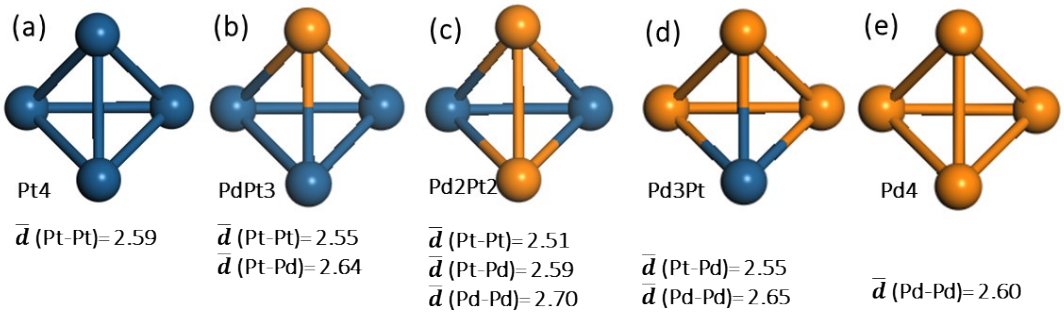

Fig. S1. Optimized structures of PtnPd(4-n) (n = 0 – 4) clusters (bond lengths in angstroms (Å) and angles in degrees (°)). Blue and orange spheres represent Pt and Pd atoms, respectively.

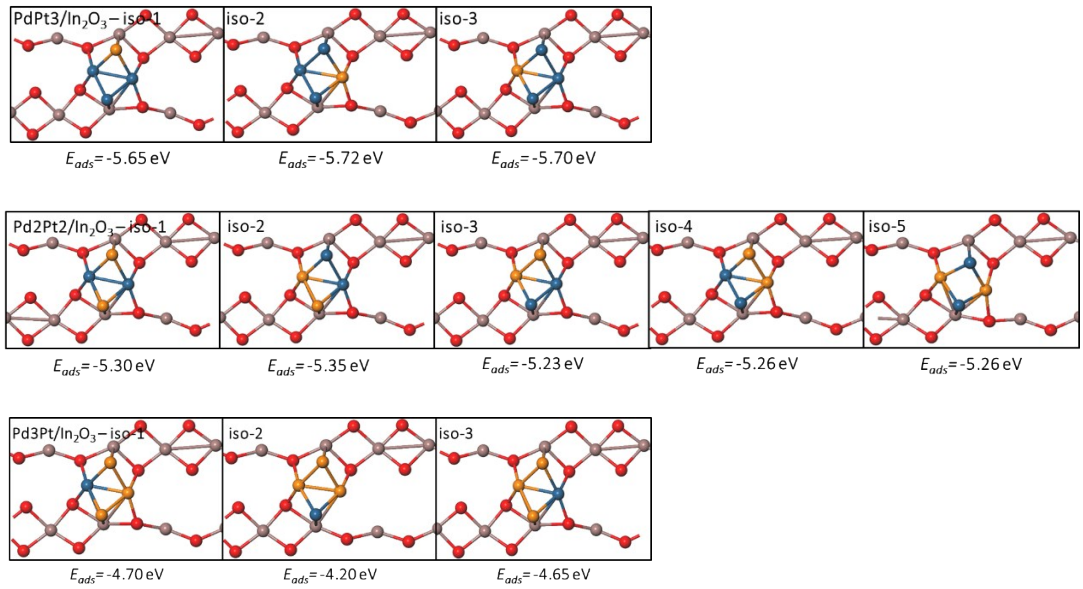

Fig. S2. Minor energy stable structures and binding energy E_{bind} of Pt3Pd/In_2O_3, Pt2Pd2/In_2O_3, and PtPd3/In_2O_3 catalysts.

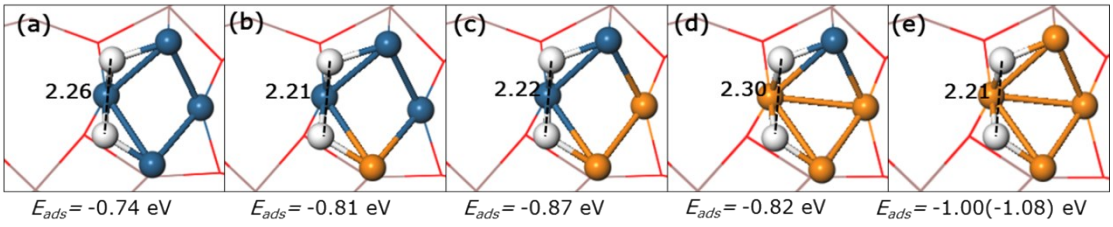

Fig. S3. The optimized structures along with adsorption energies for H_2 adsorption on PtnPd(4-n)/In_2O_3 catalysts. The data of the Pd4/In_2O_3 case in brackets are the results reported by Ye *et. al.*.[1]

References

(1) Jingyun Ye A, B.; Chang-jun, L.; Donghai, M.; Qingfeng, G. Methanol synthesis from CO_2 hydrogenation over a Pd4/In_2O_3 model catalyst: A combined DFT and kinetic study. *J. Catal.* **2014**, 317, 44-53.