A Density Functional Theory Study on the Role of Polyacetylene as a Promoter in Selective Hydrogenation of Styrene on a Pd Catalyst

Shunxin Fei, Bo Han*, Qingfan Zhang, Ming Yang and Hansong Cheng*

Sustainable Energy Laboratory, Faculty of Materials Science and Chemistry, China University of Geosciences, 388, Lumo Road, Wuhan 430074, P. R. China.

***Corresponding authors**

E-mail address: hanbo@cug.edu.cn (B. Han), chghs2@gmail.com (H. Cheng)

Tel.: +86 027 67883049; fax: +86 027 67883431.

Table S1. Bader charge analysis of the electronic rearrangement upon Pd adsorption

	type	X	Y	Z	CHARGE	MIN	ATOMIC
Pd25	Pd_4/PA	4.5968	8.5332	3.2393	9.891	1.0307	81.1384
Pd26	Pd_4/PA	4.9077	5.8752	3.3268	9.8984	1.0319	87.2486
Pd27	Pd_4/PA	3.4747	7.1618	5.2251	10.1023	1.1564	533.7344
Pd28	Pd_4/PA	5.9763	7.3728	5.2739	10.096	1.1635	546.0398
Pd25	Pd_4/PE	5.2188	9.3088	4.0953	10.0036	1.1238	88.0698
Pd26	Pd_4/PE	5.6721	6.7428	4.3966	10.0004	1.1068	120.908
Pd27	Pd_4/PE	4.2889	8.0633	6.2127	10.0142	1.149	451.9331
Pd28	Pd_4/PE	6.8138	8.4565	5.9898	10.0326	1.1295	419.8379

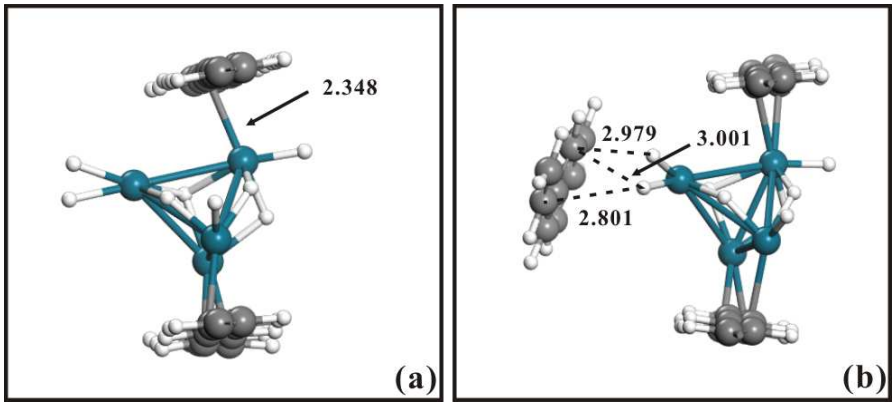

Figure S1. The optimized structures of (a) Pd_4H_8/2PA, and (b) styrene adsorbed Pd_4H_8/2PA, where the calculated styrene adsorption energy is -0.094 eV, significantly lower than the value on Pd_4H_8/PA (1.57 eV)

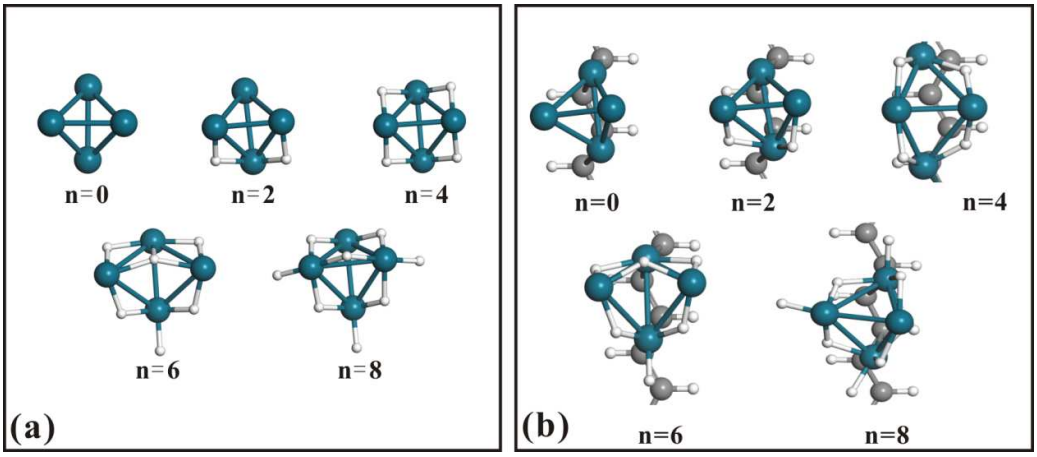

Figure S2. Optimized structure of H atoms adsorb on (a) Pd_4 cluster, and (b) Pd_4/PA cluster.

Table S2. Average bond length of Pd-Pd and Pd-H for the Pd_4 cluster and Pd_4/PA

Number of H atoms	Pd_4		Pd_4/PA	
	Pd-Pd (Å)	Pd-H (Å)	Pd-Pd (Å)	Pd-H (Å)
0	2.608	-	2.657	-
2	2.741	1.785	2.756	1.686
4	2.743	1.714	2.996	1.717
6	2.995	1.778	2.910	1.734
8	2.889	1.717	2.860	1.728

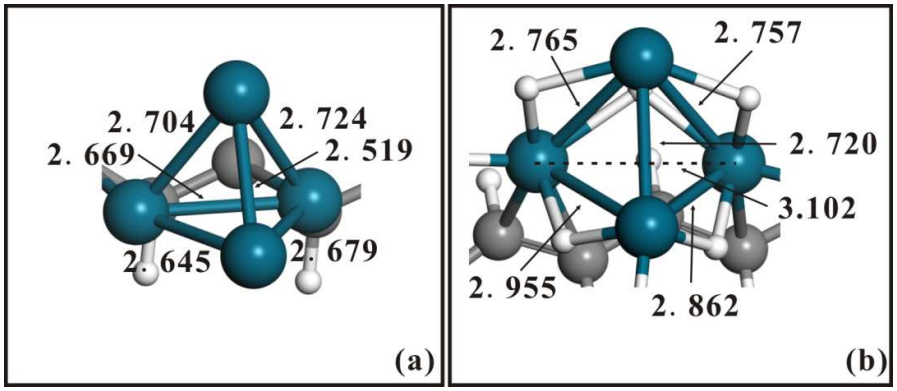

Figure S3. Optimized structure of (a) pure Pd_4 cluster on polyacetylene, (b) Pd_4H_8 supported on polyacetylene.

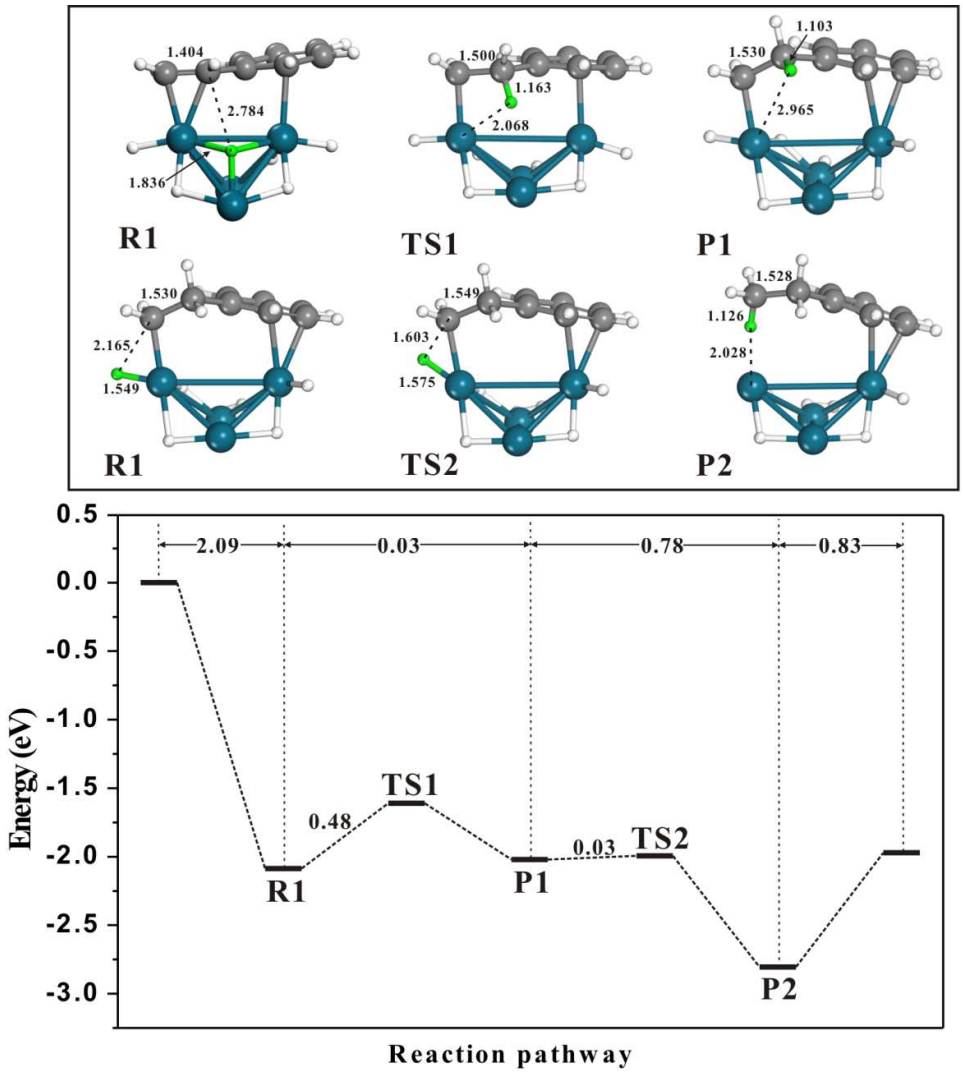

Figure S4. Calculated energy diagram of the hydrogenation process of the second route on the Pd_4H_8 cluster.

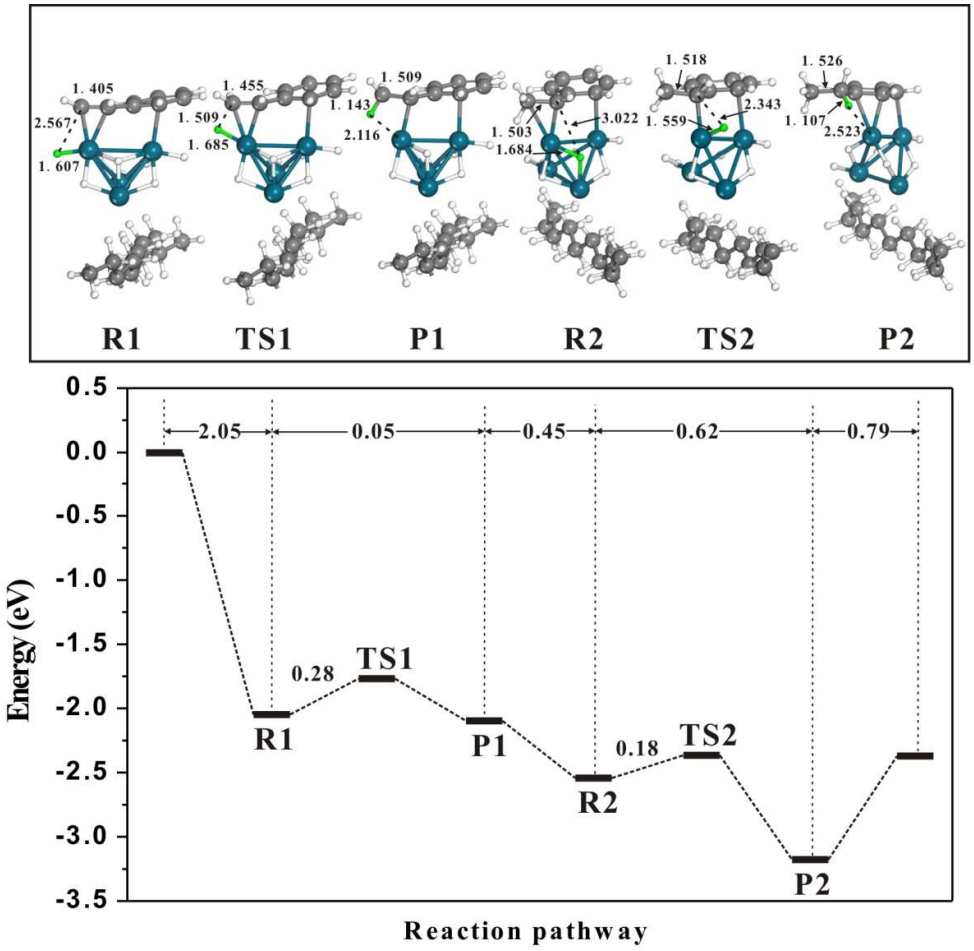

Figure S5. Calculated energy diagram of the hydrogenation process of the styrene on the Pd_4H_8/polyethylene.