

Electronic Supplementary Information

Carbon dioxide conversion to methanol on PdCo bimetallic catalyst

Huynh Tat Thanh,^{a,b,c} Ong Kim Le,^{a,b} Viorel Chihaiia,^d Do Ngoc Son,^{a,b,*}

^a Ho Chi Minh City University of Technology (HCMUT), 268 Ly Thuong Kiet Street, District 10, Ho Chi Minh City, Vietnam. E-mail: dnson@hcmut.edu.vn.

^b Vietnam National University Ho Chi Minh City, Linh Trung Ward, Ho Chi Minh City, Vietnam.

^c An Giang University, VNU-HCM, 18 Ung Van Khiem street, Dong Xuyen ward, Long Xuyen city, An Giang province.

^d Institute of Physical Chemistry "Ilie Murgulescu" of the Romanian Academy, Splaiul Independentei 202, Sector 6, 060021 Bucharest, Romania.

Table S1. Bond length of intermediates

No.	Intermediate	C-O1	C-O2	C-H1	C-H2	C-H3	CO1-H3	CO2-H4
1	CO ₂ [*]	1.18	1.18					
2	COOH [*]	1.24	1.36				0.99	
3	HCOO [*]	1.27	1.27	1.11				
4	HCOOH [*]	1.22	1.35	1.11			0.98	
5	C(OH) ₂ [*]	1.33	1.32				0.99	1.01
6	CO [*] ...H ₂ O [*]	1.18						
7	H ₂ COO [*]	1.38	1.39	1.12	1.13			
8	HCO [*] ...H ₂ O [*]	1.22		1.13				
9	COH [*] ...H ₂ O [*]	1.29					1.07	
10	H ₂ COOH [*]	1.48	1.36	1.11	1.11		0.98	
11	HC(OH) ₂ [*]	1.37	1.36	1.11			0.99	0.98
12	H ₂ CO [*] ...H ₂ O [*]	1.23		1.11	1.12			
13	H ₂ C(OH) ₂ [*]	1.40	1.43	1.11	1.10		0.98	0.99
14	HCOH [*] ...H ₂ O [*]	1.32		1.14			1.03	
15	H ₃ CO [*] ...H ₂ O [*]	1.41		1.11	1.12	1.11		
16	H ₂ COH [*] ...H ₂ O [*]	1.36		1.10	1.11		1.01	
17	CH ₃ OH [*] ...H ₂ O [*]	1.44		1.10	1.10	1.10		1.00

Note: The OH bond lengths in H₂O are not mentioned. O2 is the oxygen at higher position than O1. H1, H2, H3 in C-H1, C-H2, C-H3 are hydrogen atoms with an increasing of height, respectively. H3, H4 in CO1-H3, CO2-H4 are hydrogen atoms directly bonding to O1 and O2, respectively.

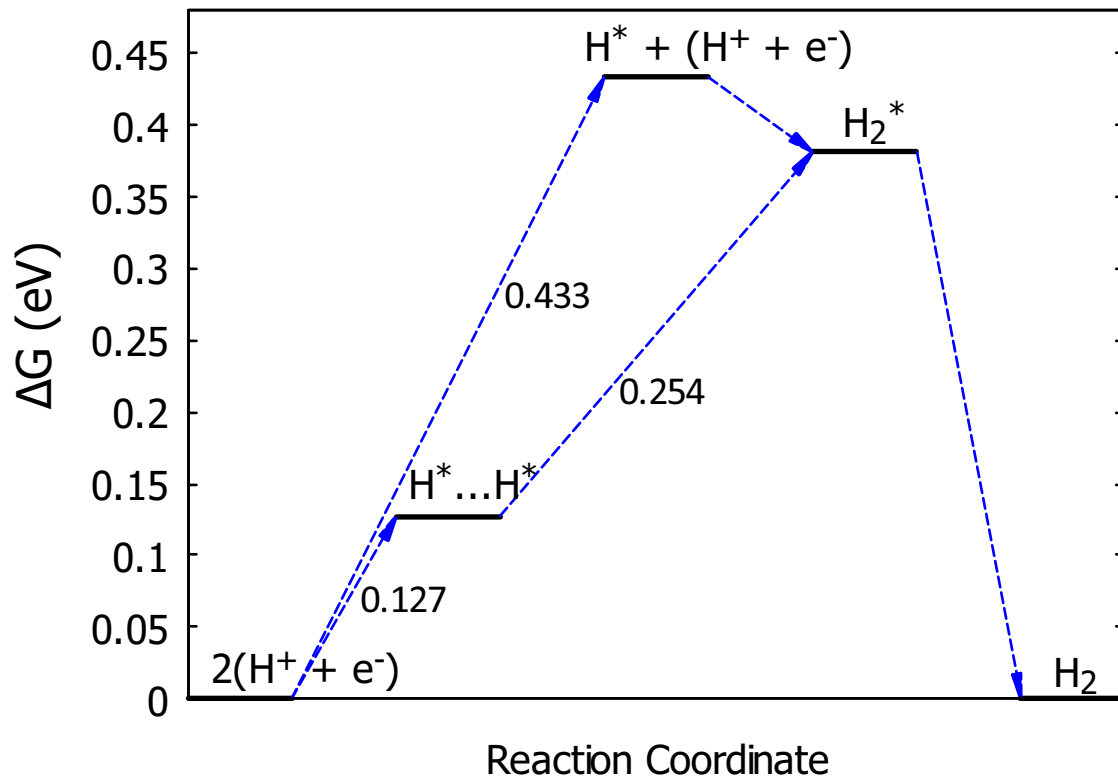


Figure S1. The free energy diagram for hydrogen evolution reaction on the PdCo alloy.

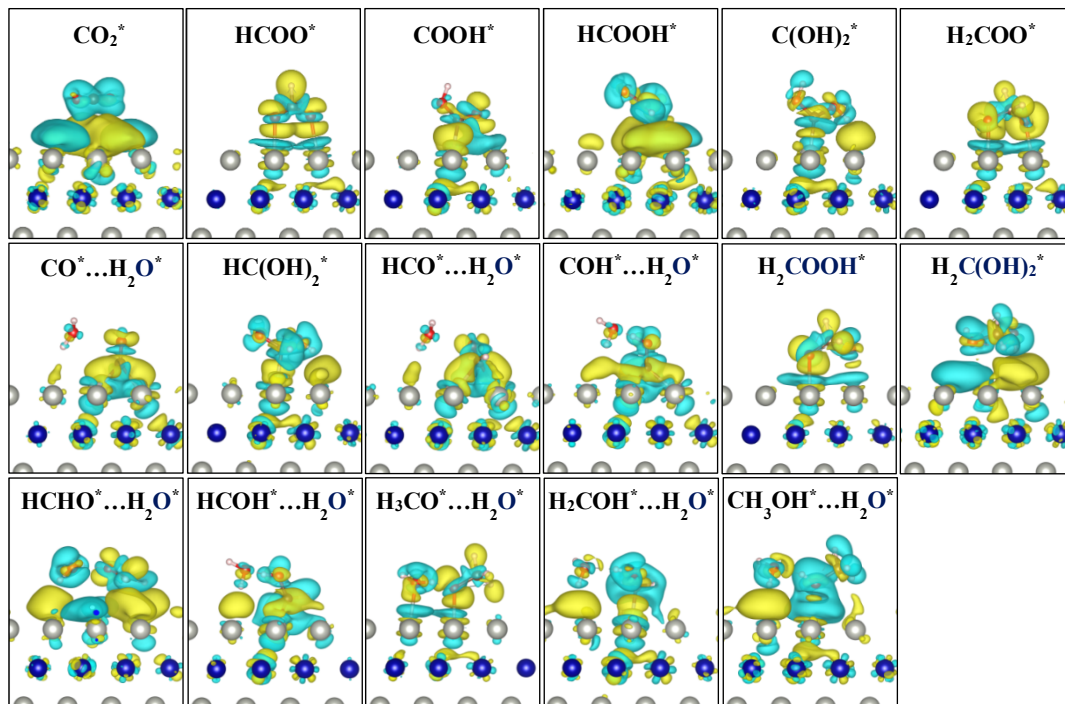


Figure S2. The CDD of intermediates. Negative charge accumulation (yellow) and negative charge donation (cyan).

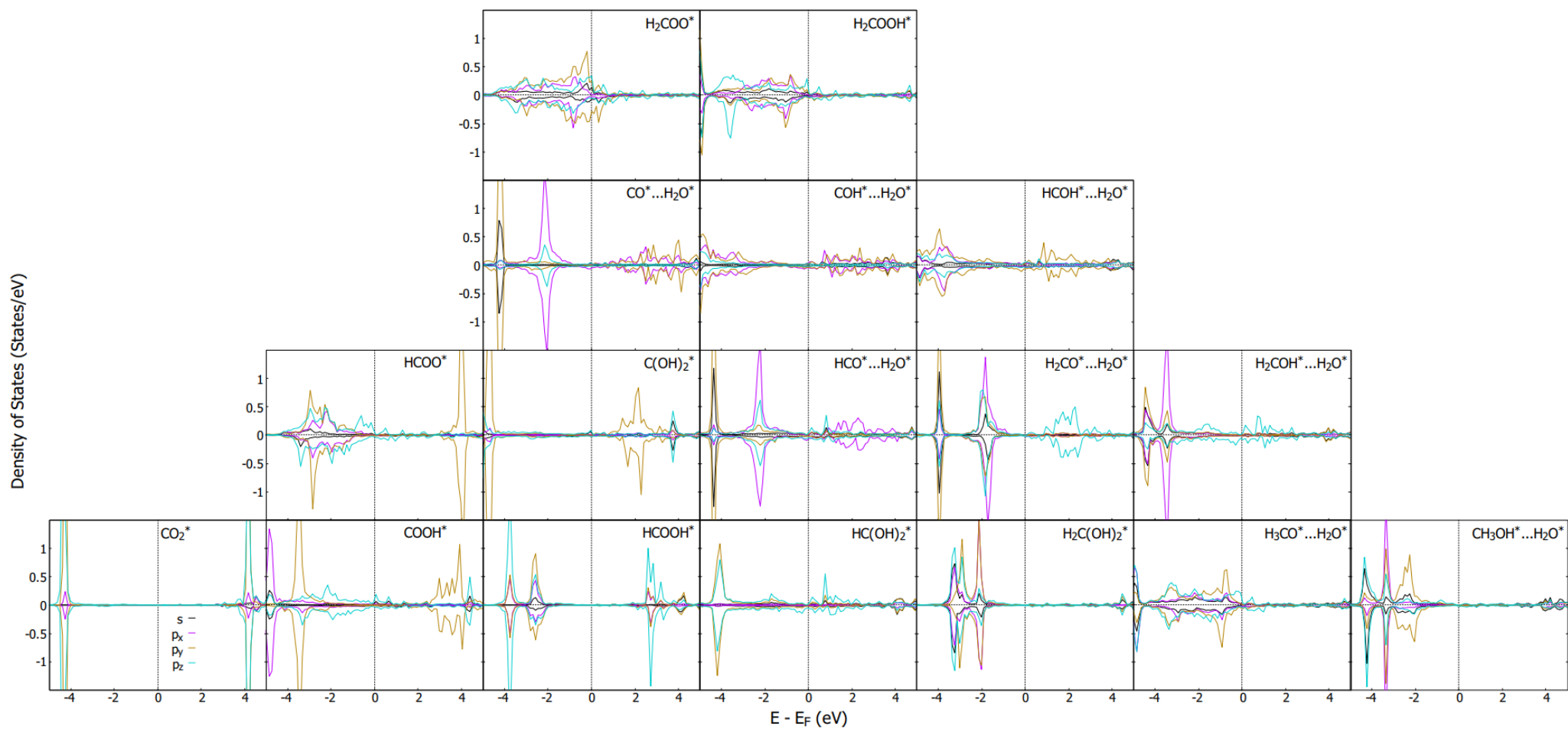


Figure S3. The PDOS of intermediates.