Supporting Information

Screening out the transition metal single atom supported on onion-like carbon (OLC) for the hydrogen evolution reaction

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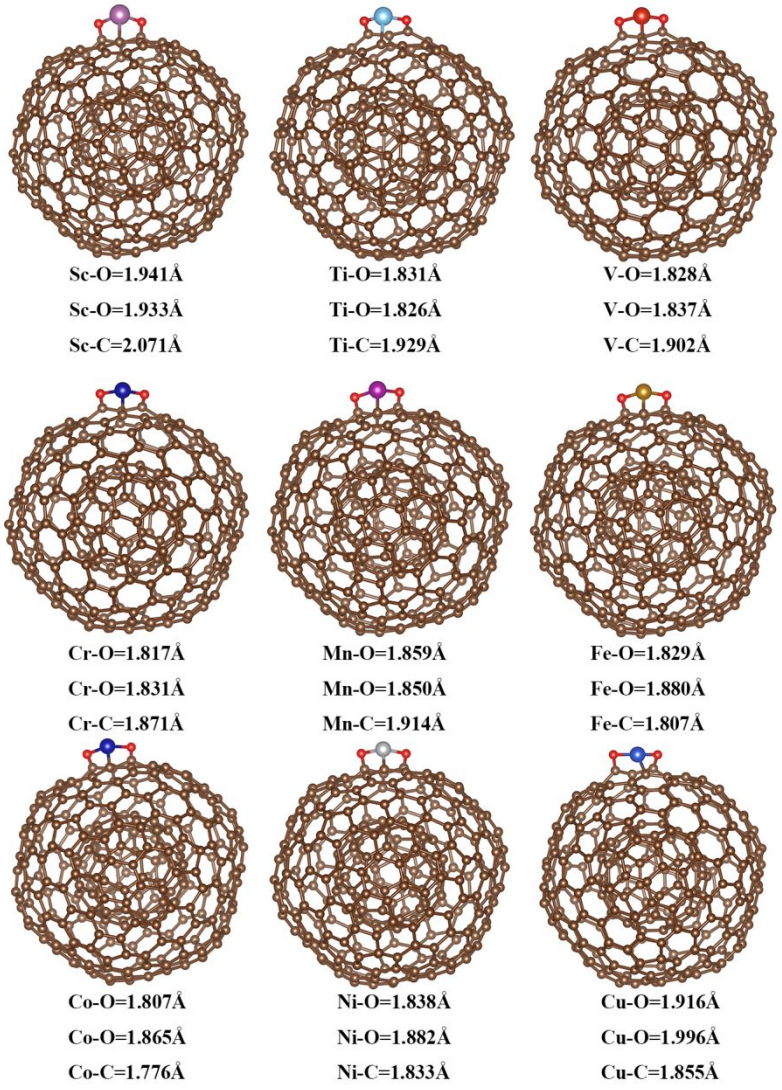

Figure S1. The relaxed geometries of free 3d TM_1/OLC complexes (TM=Sc-Cu).

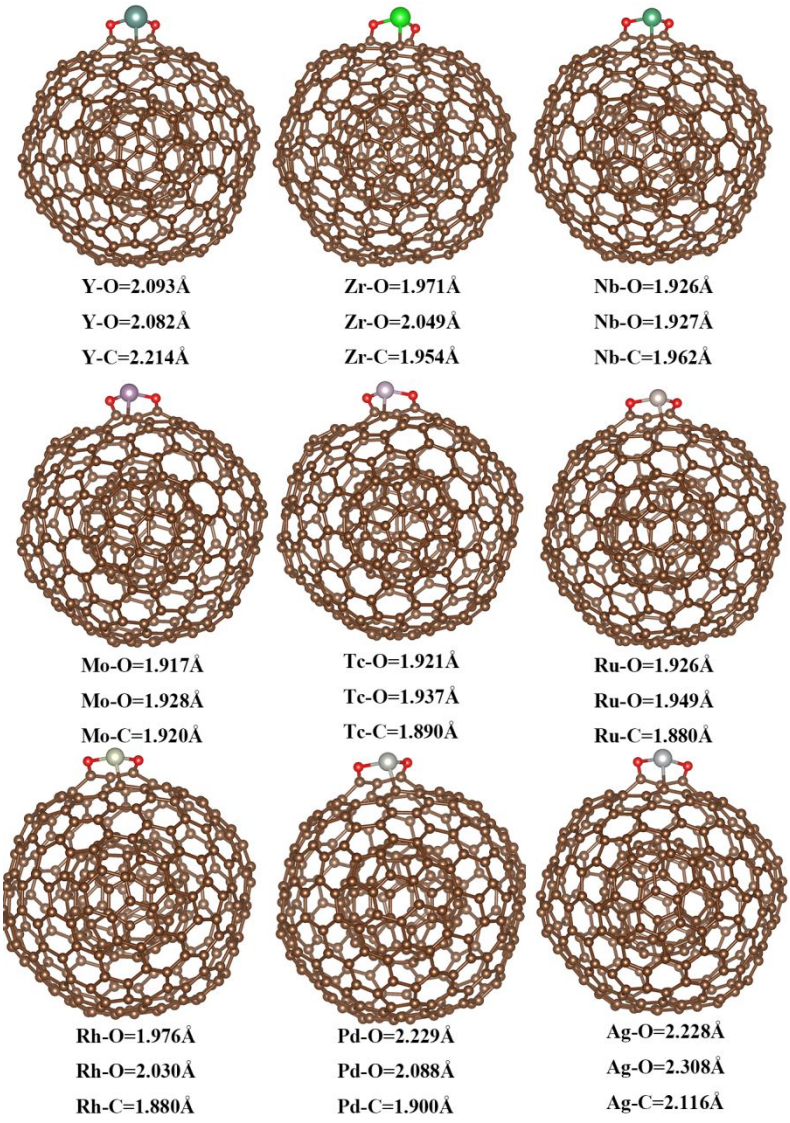

Figure S2. The relaxed geometries of free 4d TM_1/OLC complexes (TM=Y-Ag).

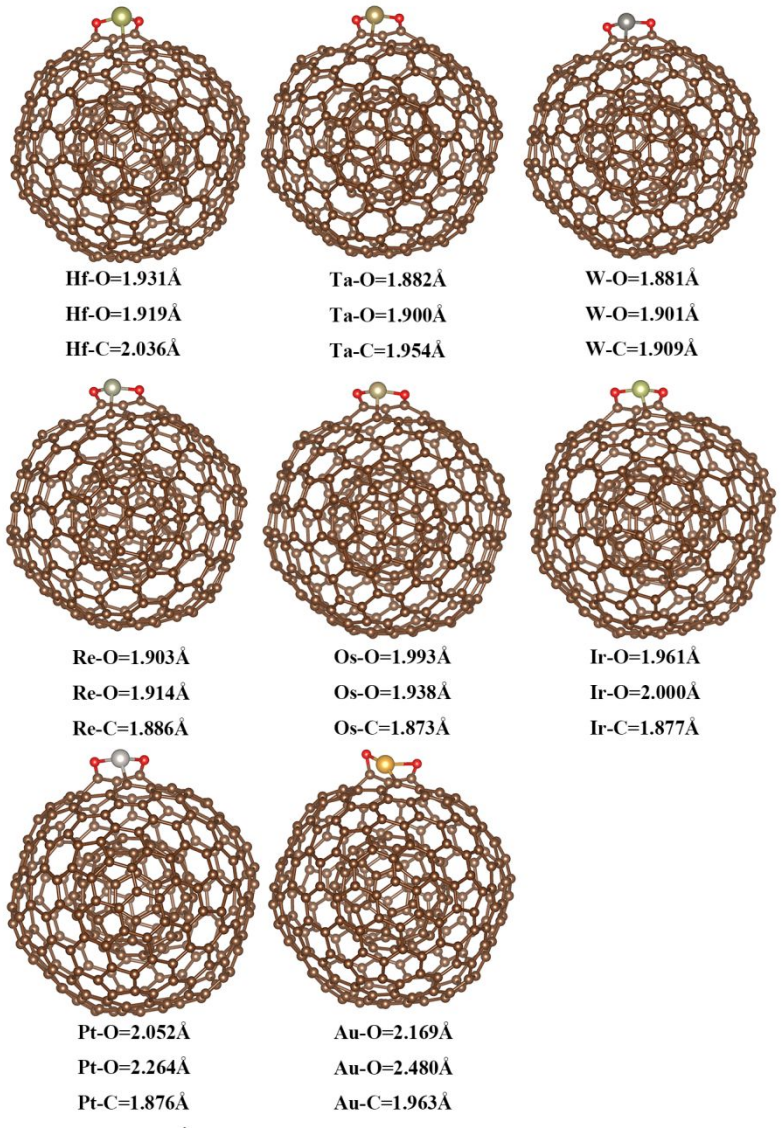

Figure S3. The relaxed geometries of free 5d TM_1/OLC complexes (TM=Hf-Au).

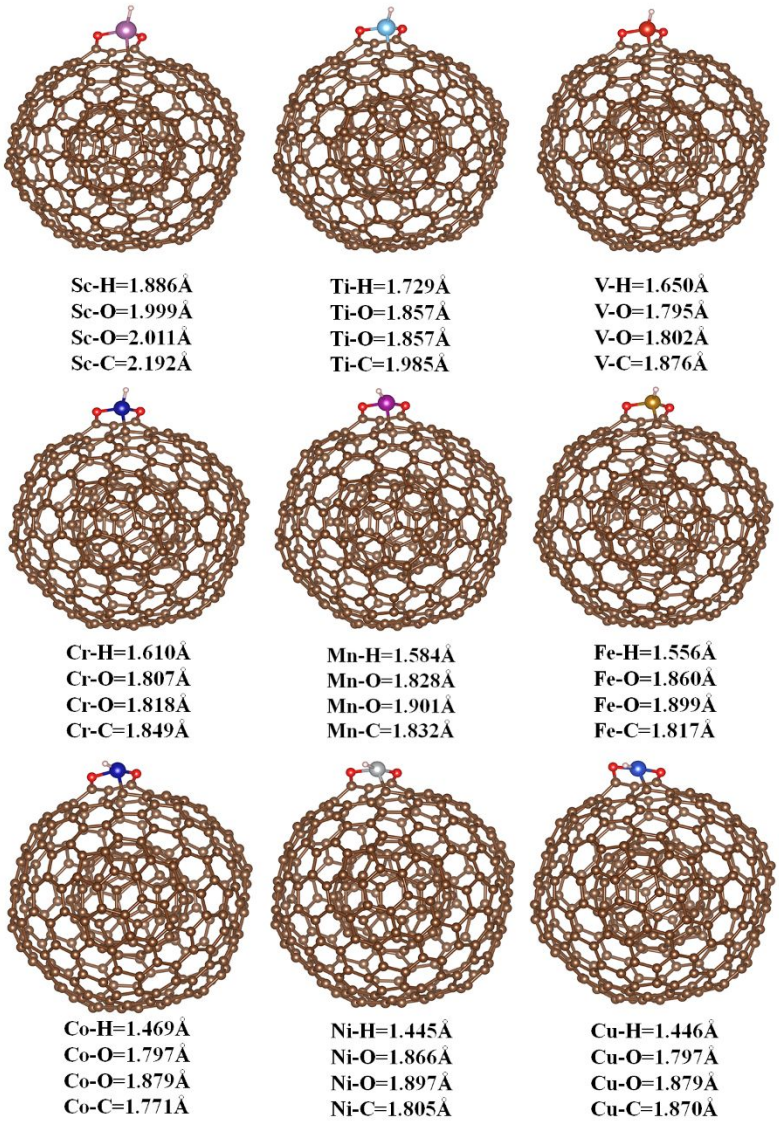

Figure S4. The relaxed geometries of 3d TM_1/OLC complexes (TM=Sc-Cu) with one hydrogen adsorption.

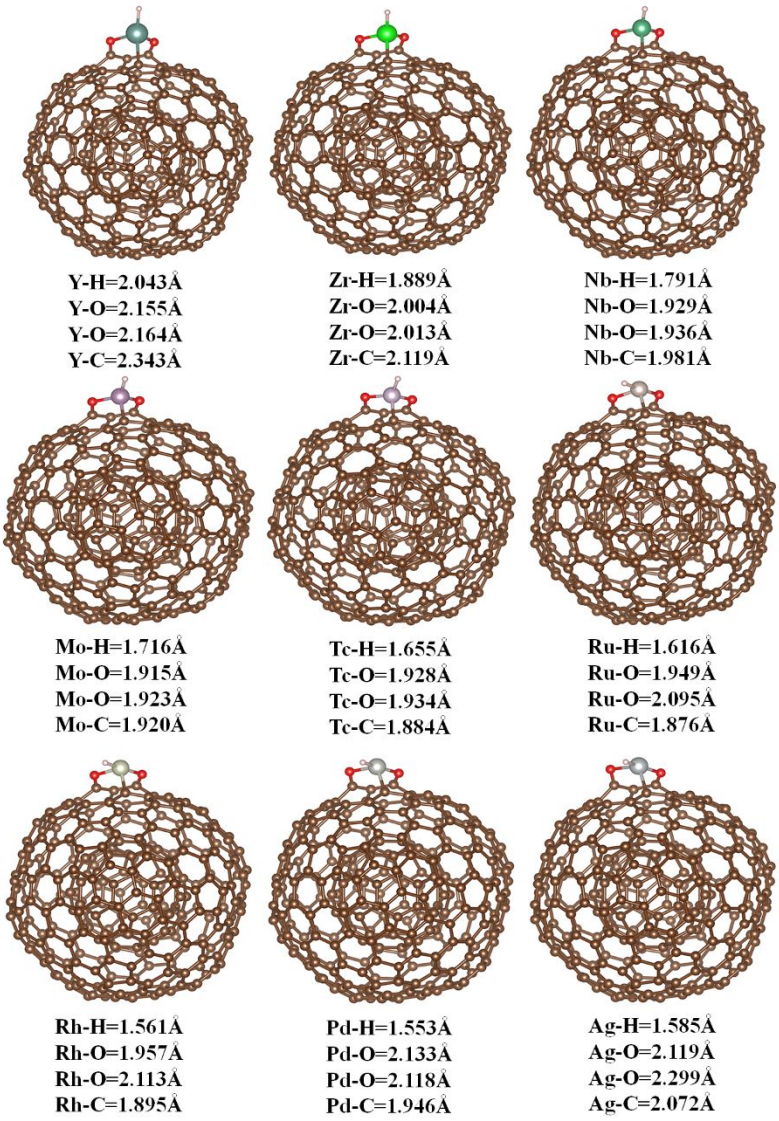

Figure S5. The relaxed geometries of 4d TM_1/OLC complexes (TM=Y-Ag) with one hydrogen adsorption.

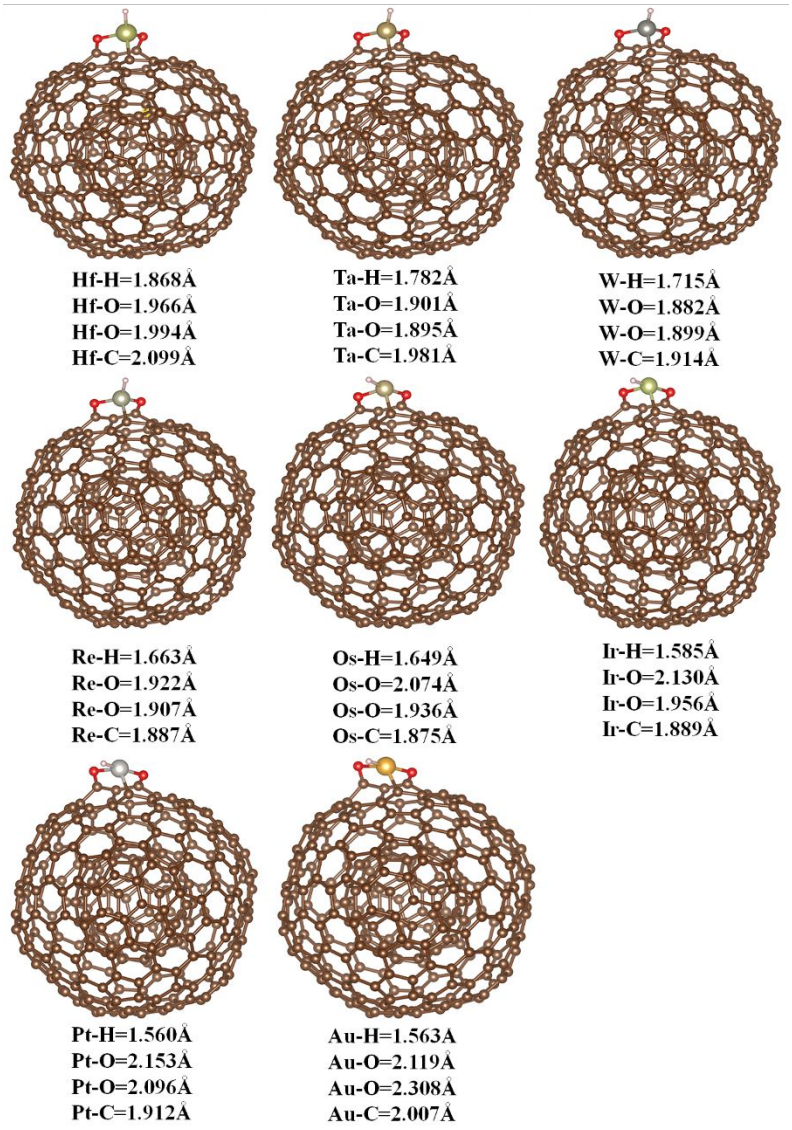

Figure S6. The relaxed geometries of 5d TM_1/OLC complexes (TM=Hf-Au) with one hydrogen adsorption.

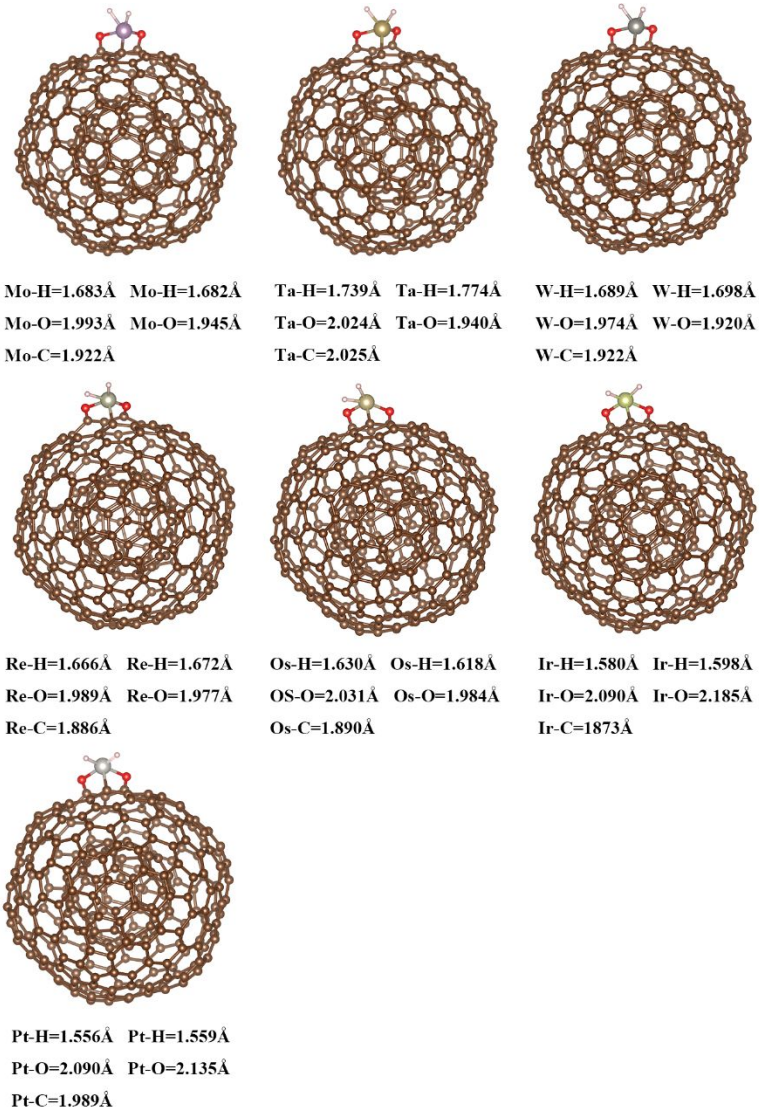

Figure S7. The relaxed geometries of TM_1/OLC complexes (TM=Mo, Ta, W, Re, Os, Ir, and Pt) with 2nd hydrogen adsorption.

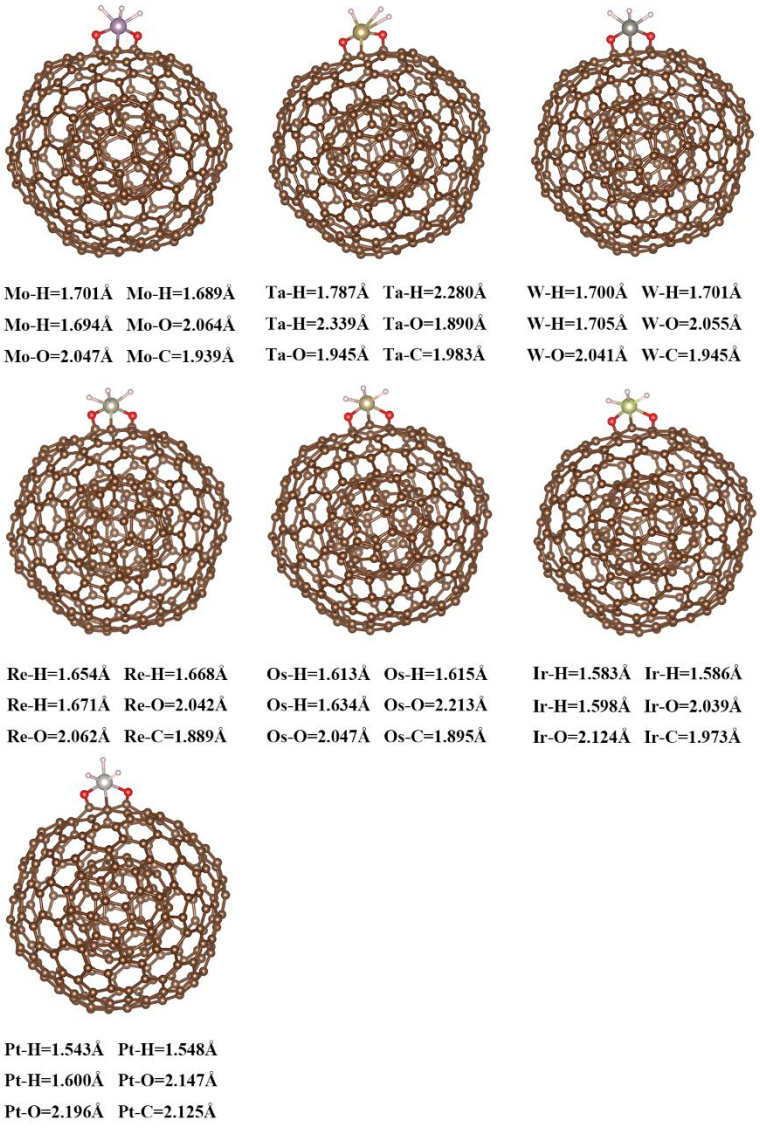

Figure S8. The relaxed geometries of TM_1/OLC complexes (TM=Mo, Ta, W, Re, Os, Ir, and Pt) with 3rd hydrogen adsorption.

Table S1. The binding energies (E_b) of TM_1/OLC species, the difference between binding energy and cohesion energy (E_{coh}) of TM, and Mulliken charge of TM.

Species	E_b (eV)	E_b-E_{coh} (eV)	Q (M) (|e|)
Sc	11.67	7.77	1.32
Ti	11.29	6.44	1.54
V	10.34	5.03	1.40
Cr	7.81	3.71	1.15
Mn	7.35	4.43	1.19
Fe	7.36	3.08	1.09
Co	7.90	3.51	0.85
Ni	7.92	3.48	0.85
Cu	6.19	2.70	0.71
Y	10.65	6.28	1.59
Zr	11.98	5.73	1.88
Nb	12.08	4.51	1.52
Mo	7.97	1.15	1.25
Tc	8.84	1.99	1.04
Ru	8.67	1.93	0.79
Rh	7.36	1.61	0.89
Pd	5.42	1.53	0.64
Ag	3.67	0.72	0.67
Hf	11.65	5.21	1.88
Ta	11.31	3.21	1.65

W	13.65	4.75	1.45
Re	9.55	1.52	1.21
Os	7.82	-0.35	0.98
Ir	7.96	1.02	1.06
Pt	6.35	0.51	0.74
Au	4.35	0.54	0.44

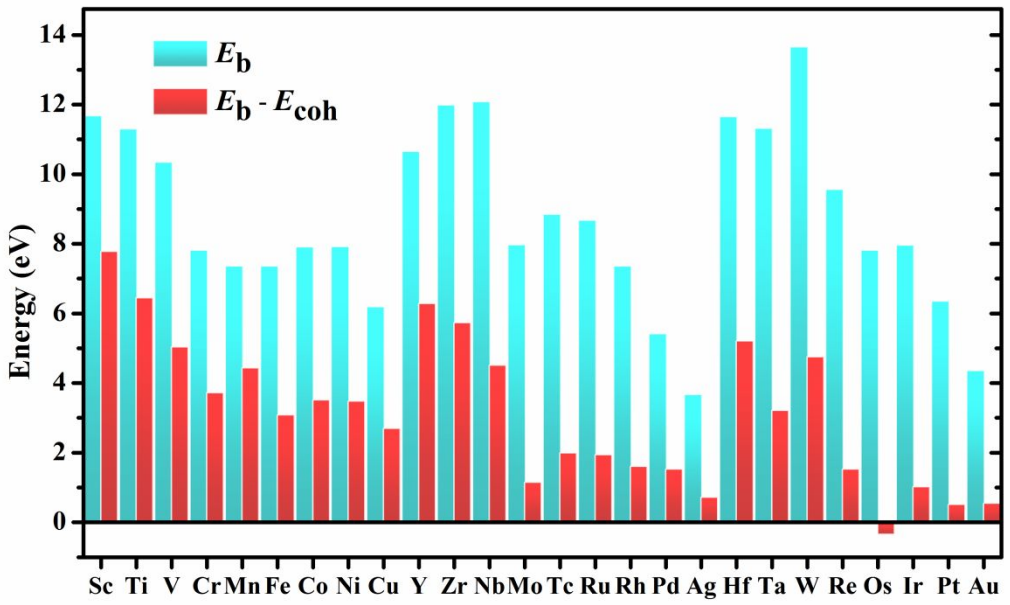

Figure S9. The binding energies (E_b) of TM_1/OLC species, the difference between binding energy energy and cohesion energy (E_{coh}) of TM were also given, in which the positive values (E_b-E_{coh}) indicate that E_b values are higher than E_{coh}.

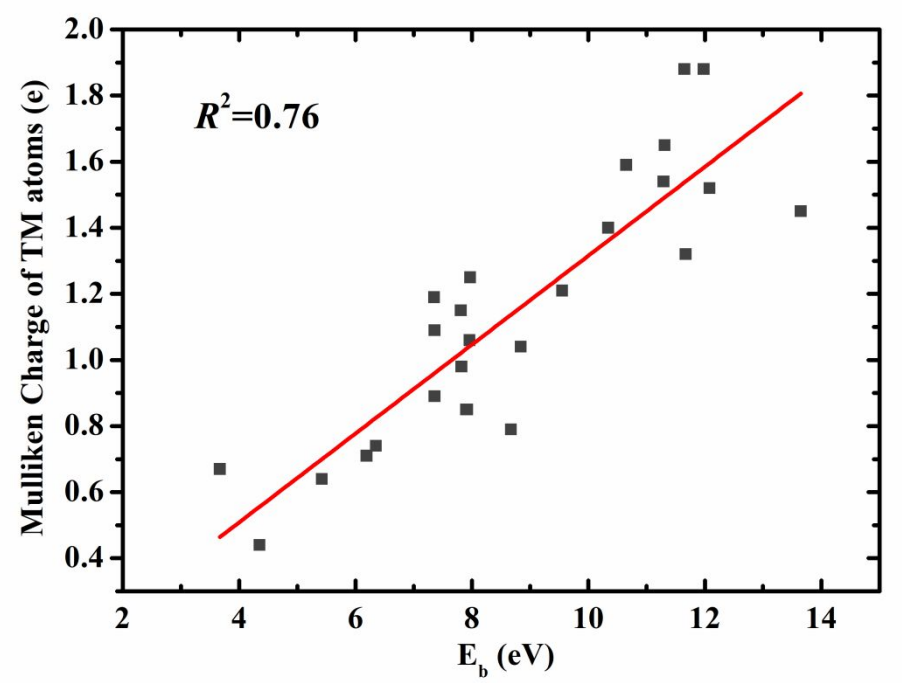

Figure S10. The linear relation between the binding energies (E_b) of TM_1/OLC and Mulliken charges of TM atoms.

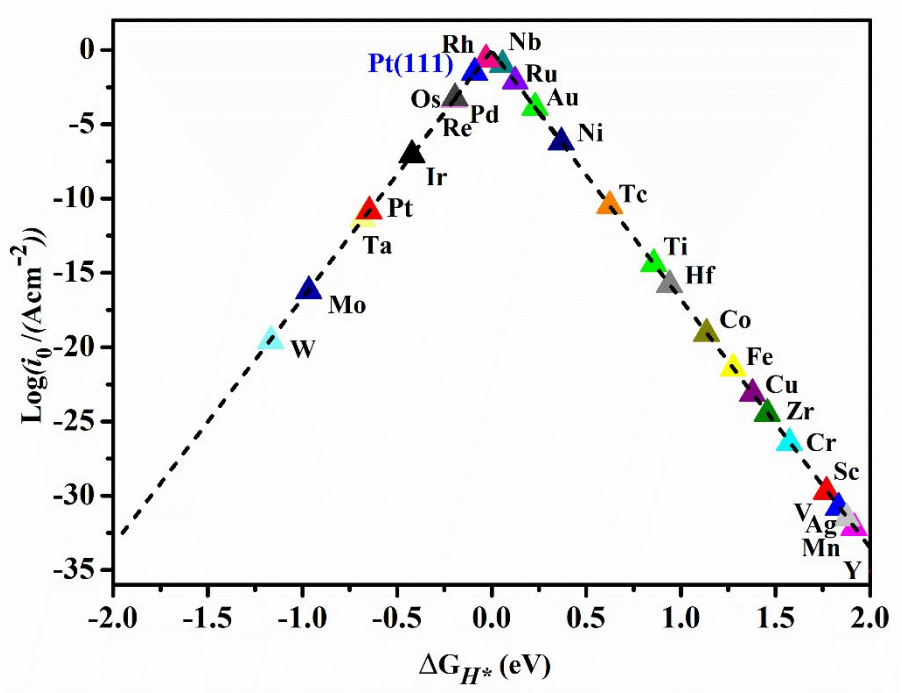

Figure S11. Volcanic curve of the exchange current (i_0) as a function of the average ΔG_{H^*} of TM supported OLC with one H adsorbed.

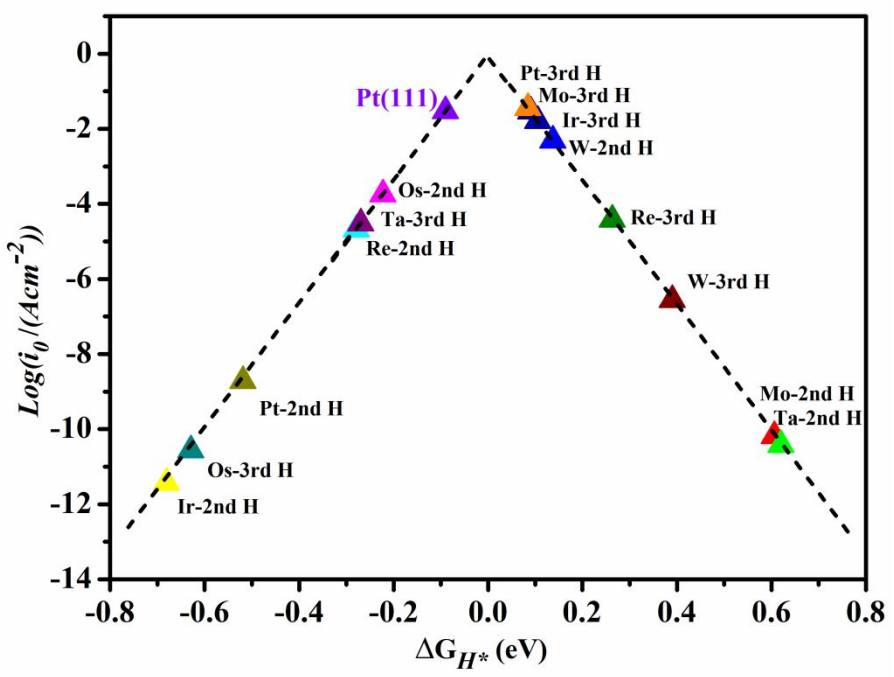

Figure S12. Volcanic curve of the exchange current (i_0) as a function of the average ΔG_{H^*} of TM supported OLC with 2nd or 3rd H adsorbed.

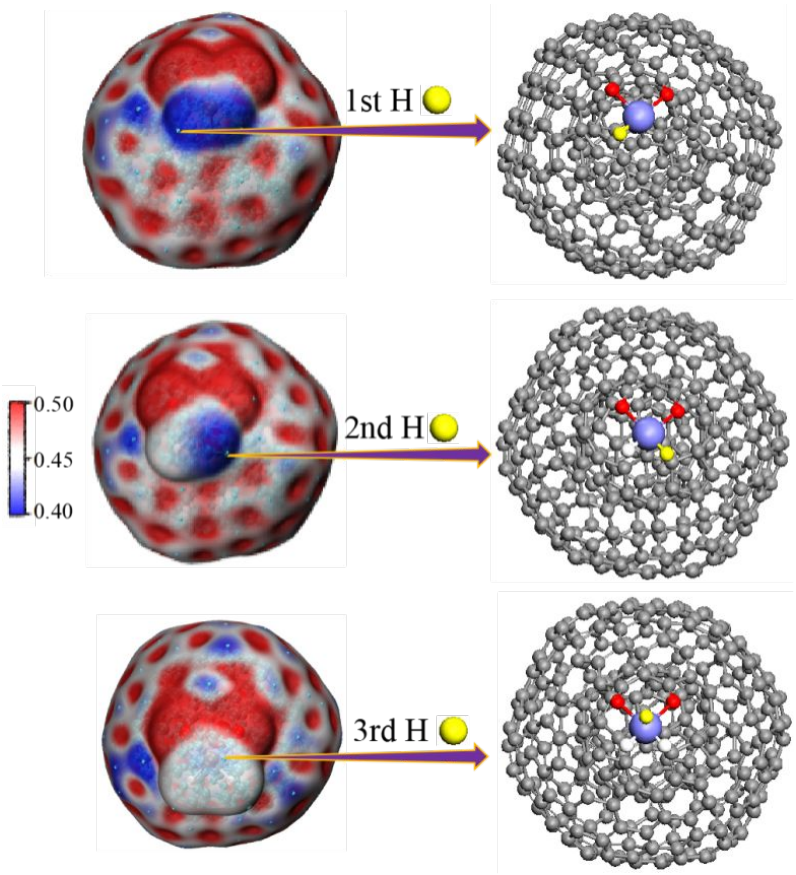

Figure S13. ALIE maps on the vdW surface of Pt_1/OLC with H adsorbed.