Supporting Information

Hägg Carbide Surfaces Induced Pt Morphological Changes: A Theoretical Insight

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Table S1. The comparison of average aggregation energies of the gas phase Ptn isomers calculated at Monkhorst-Pack and Gamma points.

Pt_{gas}	E_{agg}		ΔE_{agg}
	Gamma	M-P	
Pt_2	-1.9517	-1.9514	-0.0003
Pt_3-1	-2.4877	-2.4954	0.0077
Pt_3-2	-2.3250	-2.3252	0.0002
Pt_4-1	-2.7967	-2.7964	-0.0003
Pt_4-2	-2.7722	-2.7731	0.0008
Pt_5-1	-3.0570	-3.0567	-0.0003
Pt_5-2	-3.0239	-3.0230	-0.0010
Pt_5-3	-3.0084	-3.0082	-0.0003
Pt_6-1	-3.3090	-3.3080	-0.0011
Pt_6-2	-3.1979	-3.1976	-0.0003
Pt_6-3	-3.1654	-3.1652	-0.0003
Pt_6-4	-3.1598	-3.1595	-0.0004
Pt_6-5	-3.0563	-3.0558	-0.0005
Pt_7-1	-3.3691	-3.3688	-0.0003
Pt_7-2	-3.3395	-3.3391	-0.0004
Pt_7-3	-3.3164	-3.3161	-0.0003
Pt_7-4	-3.3100	-3.3100	0.0000
Pt_7-5	-3.2867	-3.2863	-0.0003
Pt_7-6	-3.2693	-3.2687	-0.0006
Pt_7-7	-3.2501	-3.2495	-0.0006
Pt_7-8	-3.2453	-3.2449	-0.0005
Pt_8-1	-3.4935	-3.4932	-0.0003
Pt_8-2	-3.4684	-3.4681	-0.0003
Pt_8-3	-3.4572	-3.4569	-0.0003
Pt_8-4	-3.4365	-3.4357	-0.0009
Pt_8-5	-3.4157	-3.4151	-0.0006
Pt_8-6	-3.4045	-3.4045	0.0000
Pt_8-7	-3.4008	-3.4008	-0.0001
Pt_9-1	-3.6522	-3.6540	0.0018
Pt_9-2	-3.6460	-3.6460	0.0000
Pt_9-3	-3.6271	-3.6268	-0.0003
Pt_9-4	-3.5734	-3.5733	-0.0001
Pt_9-5	-3.5663	-3.5659	-0.0004
Pt_9-6	-3.5439	-3.5467	0.0029
Pt_9-7	-3.4808	-3.4803	-0.0006
Pt_{10}-1	-3.8008	-3.8005	-0.0003
Pt_{10}-2	-3.6749	-3.6744	-0.0005
Pt_{10}-3	-3.6231	-3.6236	0.0005

Pt_{10}-4	-3.5999	-3.5994	-0.0005
Pt_{10}-5	-3.5950	-3.5947	-0.0004
Pt_{10}-6	-3.5783	-3.5779	-0.0003
Pt_{11}-1	-3.7962	-3.7959	-0.0003
Pt_{11}-2	-3.7713	-3.7708	-0.0005
Pt_{11}-3	-3.7668	-3.7662	-0.0006
Pt_{11}-4	-3.6705	-3.6702	-0.0003
Pt_{12}-1	-3.8620	-3.8615	-0.0006
Pt_{12}-2	-3.8543	-3.8538	-0.0006
Pt_{12}-3	-3.8316	-3.8313	-0.0003
Pt_{12}-4	-3.8131	-3.8125	-0.0005
Pt_{12}-5	-3.8103	-3.8098	-0.0005
Pt_{12}-6	-3.7808	-3.7802	-0.0006
Pt_{12}-7	-3.7749	-3.7747	-0.0003
Pt_{12}-8	-3.7490	-3.7487	-0.0003

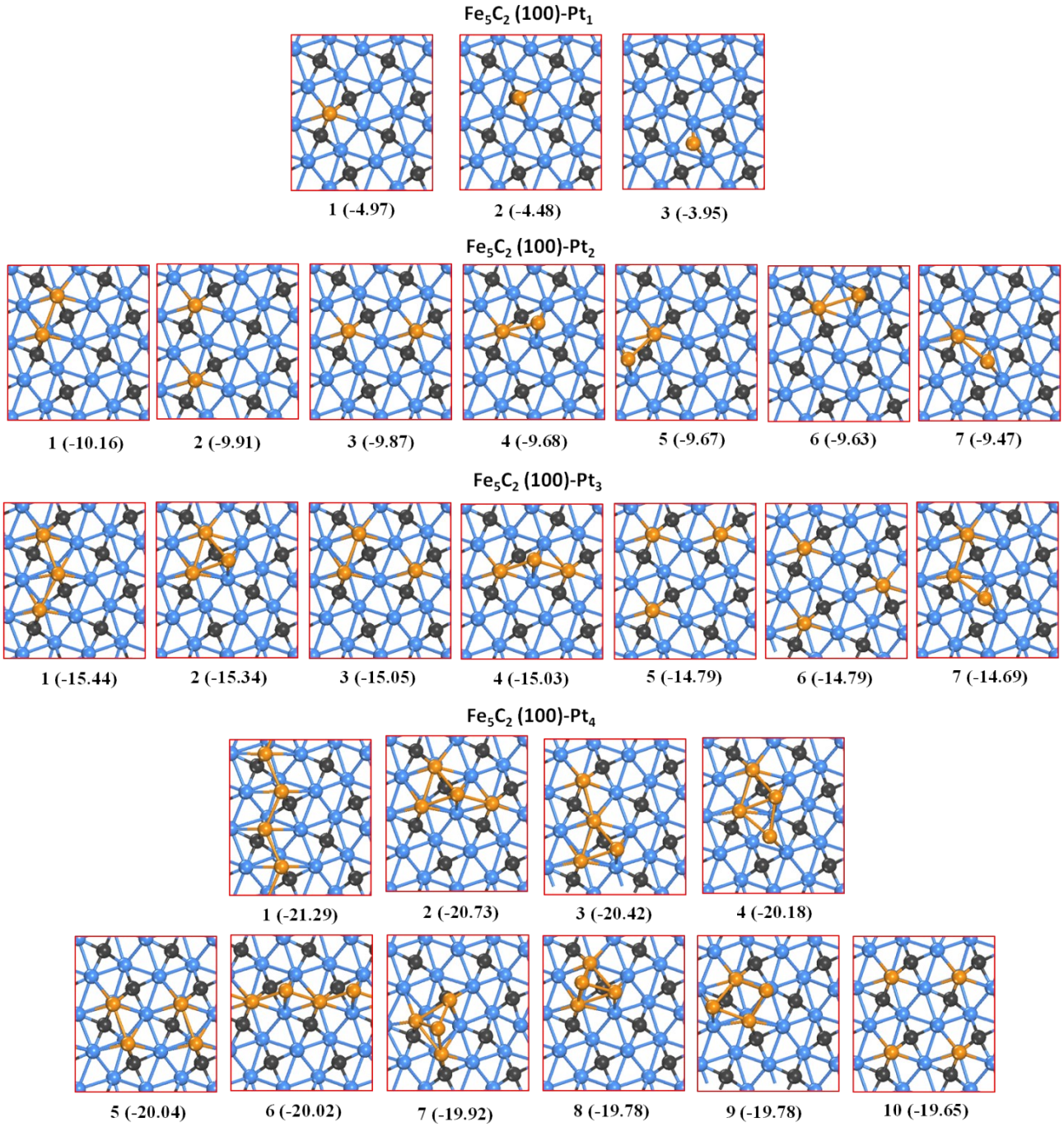

Figure S1. Various structures and adsorption energies for Pt_n (n = 1–4) on the Fe_5C_2 (100) surface (adsorption energy in eV)

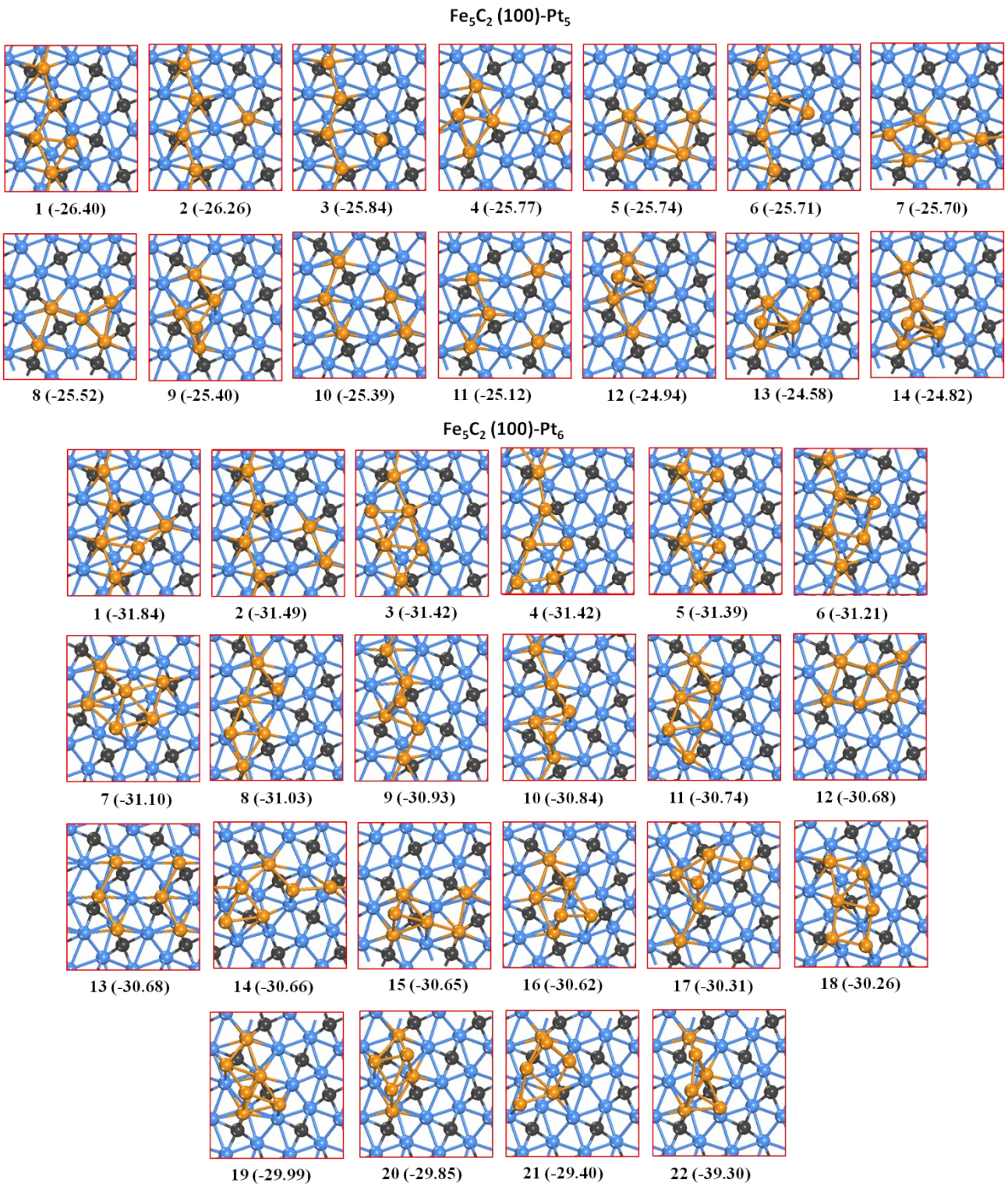

Figure S2. Various structures and adsorption energies for Pt_n (n = 5, 6) on the Fe_5C_2 (100) surface (adsorption energy in eV)

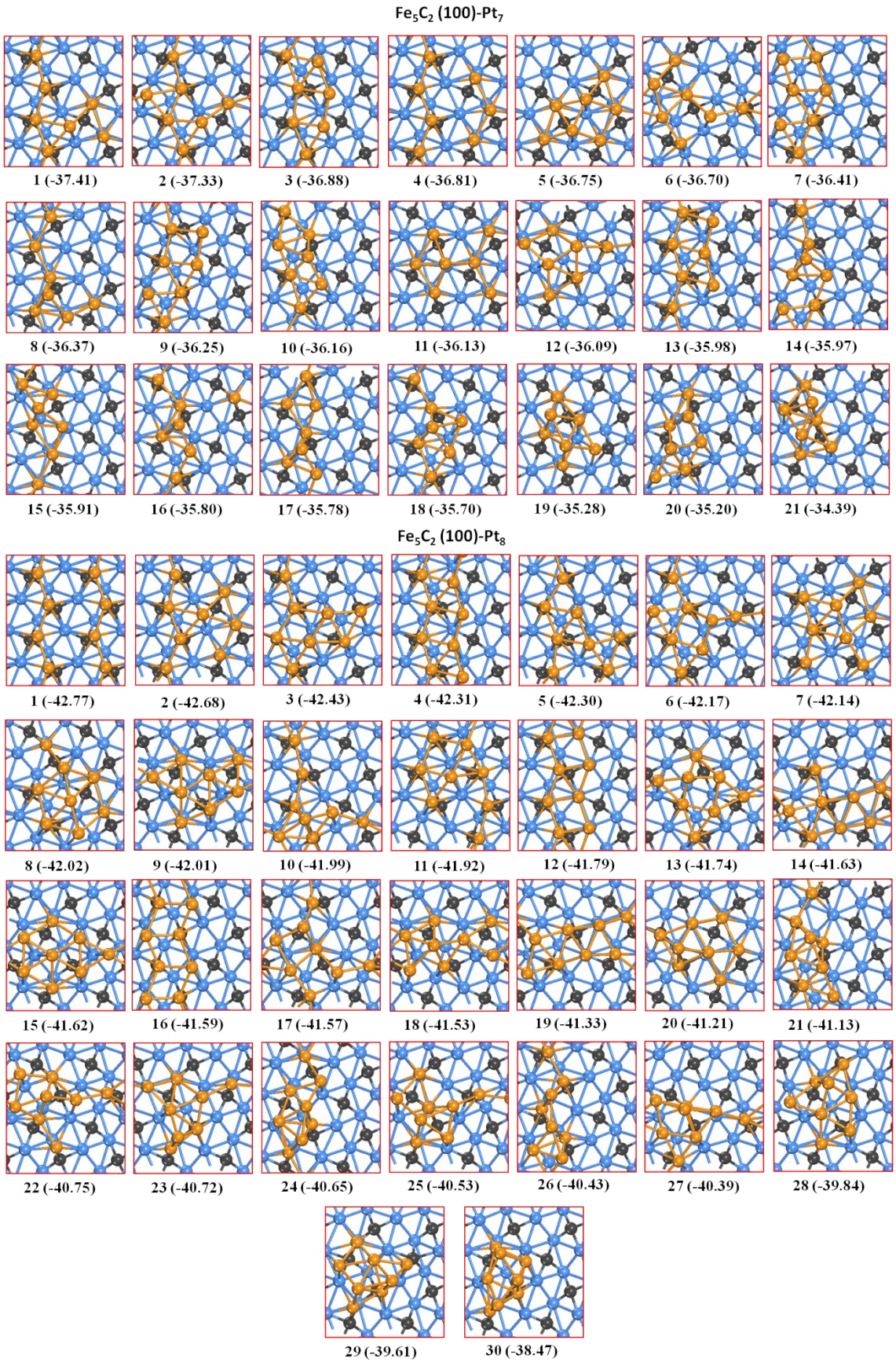

Figure S3. Various structures and adsorption energies for Pt_n (n = 7, 8) on the Fe_5C_2 (100) surface (adsorption energy in eV)

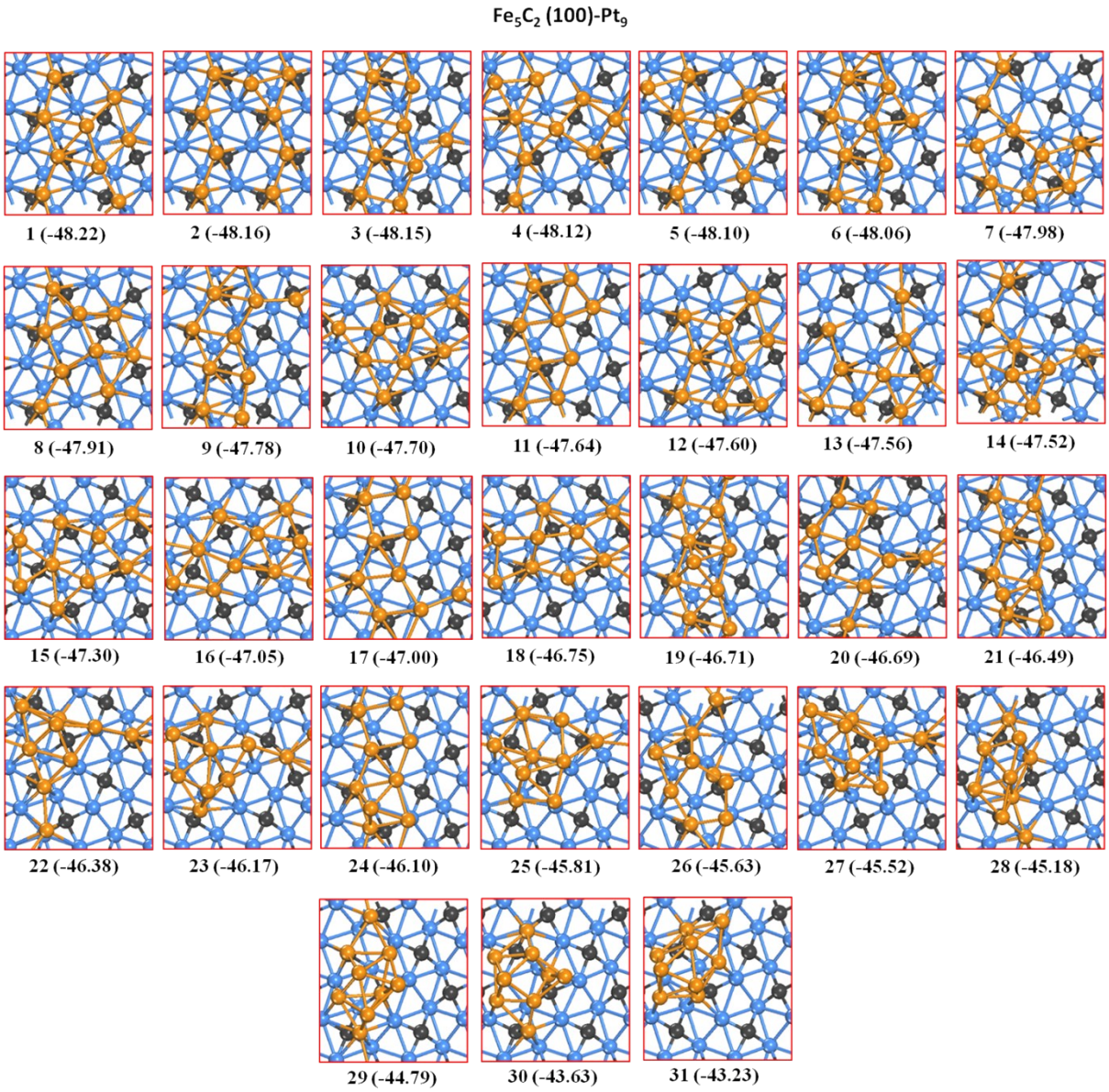

Figure S4. Various structures and adsorption energies for Pt_9 on the Fe_5C_2 (100) surface (adsorption energy in eV)

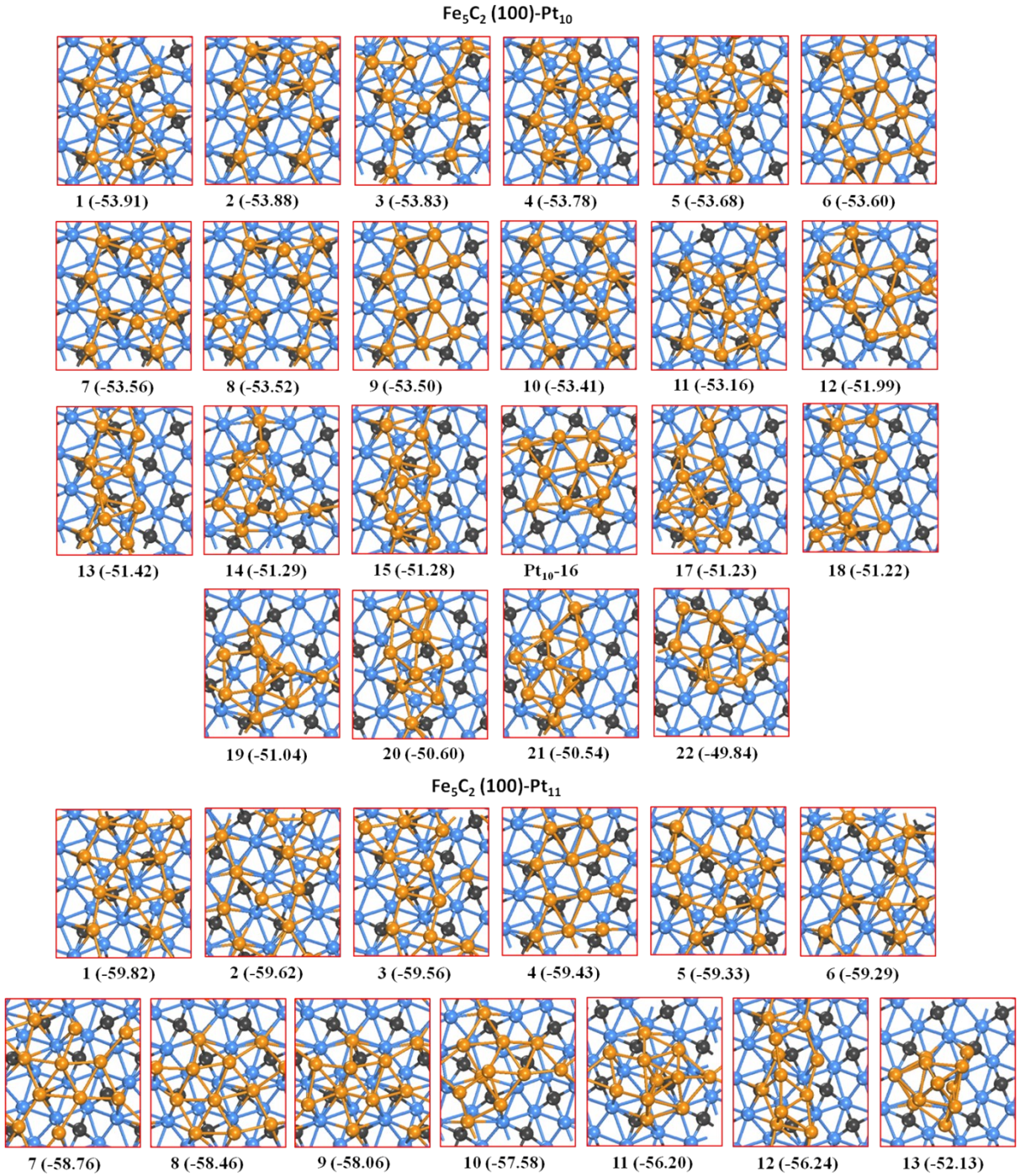

Figure S5. Various structures and adsorption energies for Pt_n (n = 10, 11) on the Fe_5C_2 (100) surface (adsorption energy in eV)

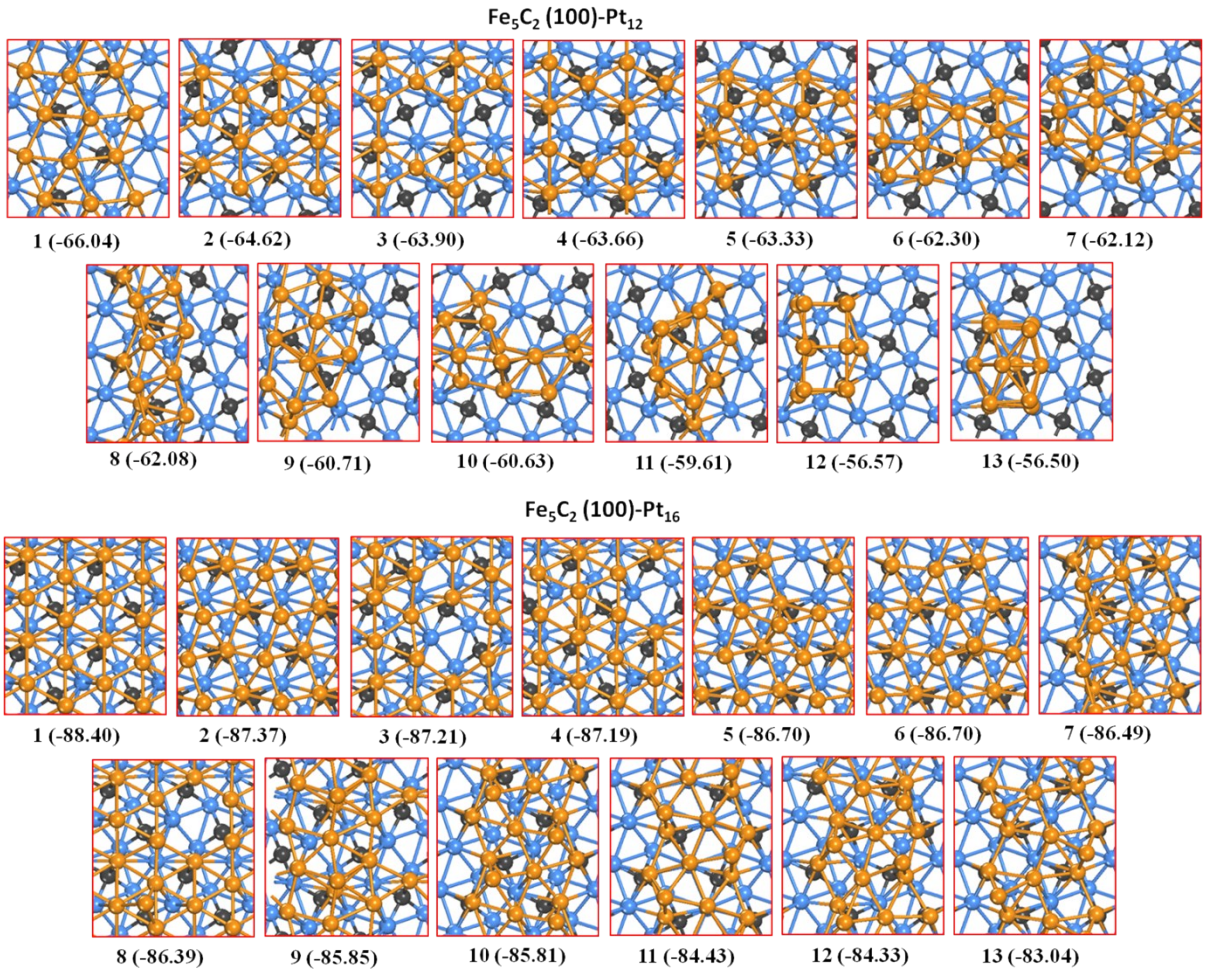

Figure S6. Various structures and adsorption energies for Pt_n (n = 12, 16) on the Fe_5C_2 (100) surface (adsorption energy in eV)

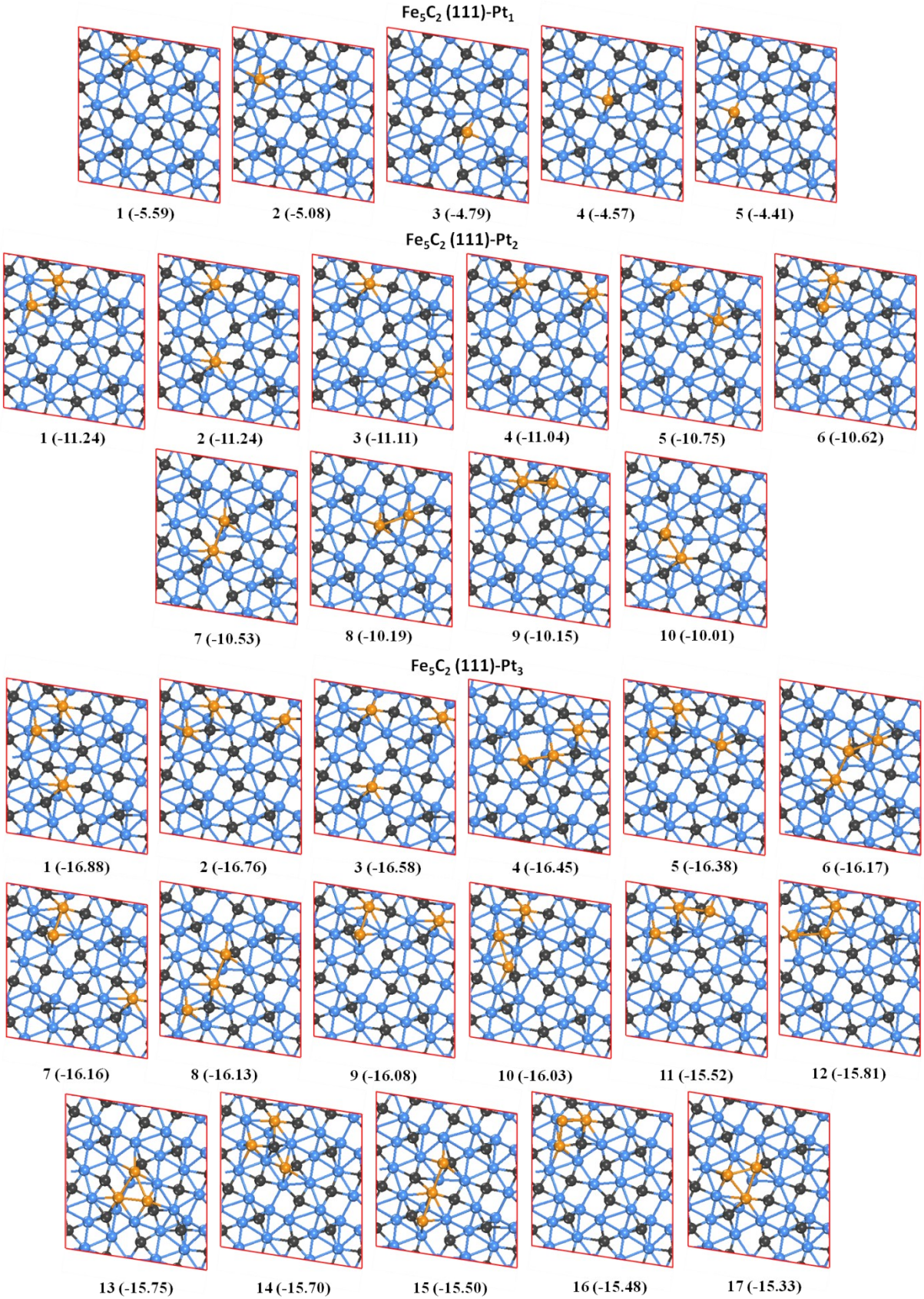

Figure S7. Various structures and adsorption energies for Pt_n (n = 1–3) on the Fe_5C_2 (111) surface (adsorption energy in eV)

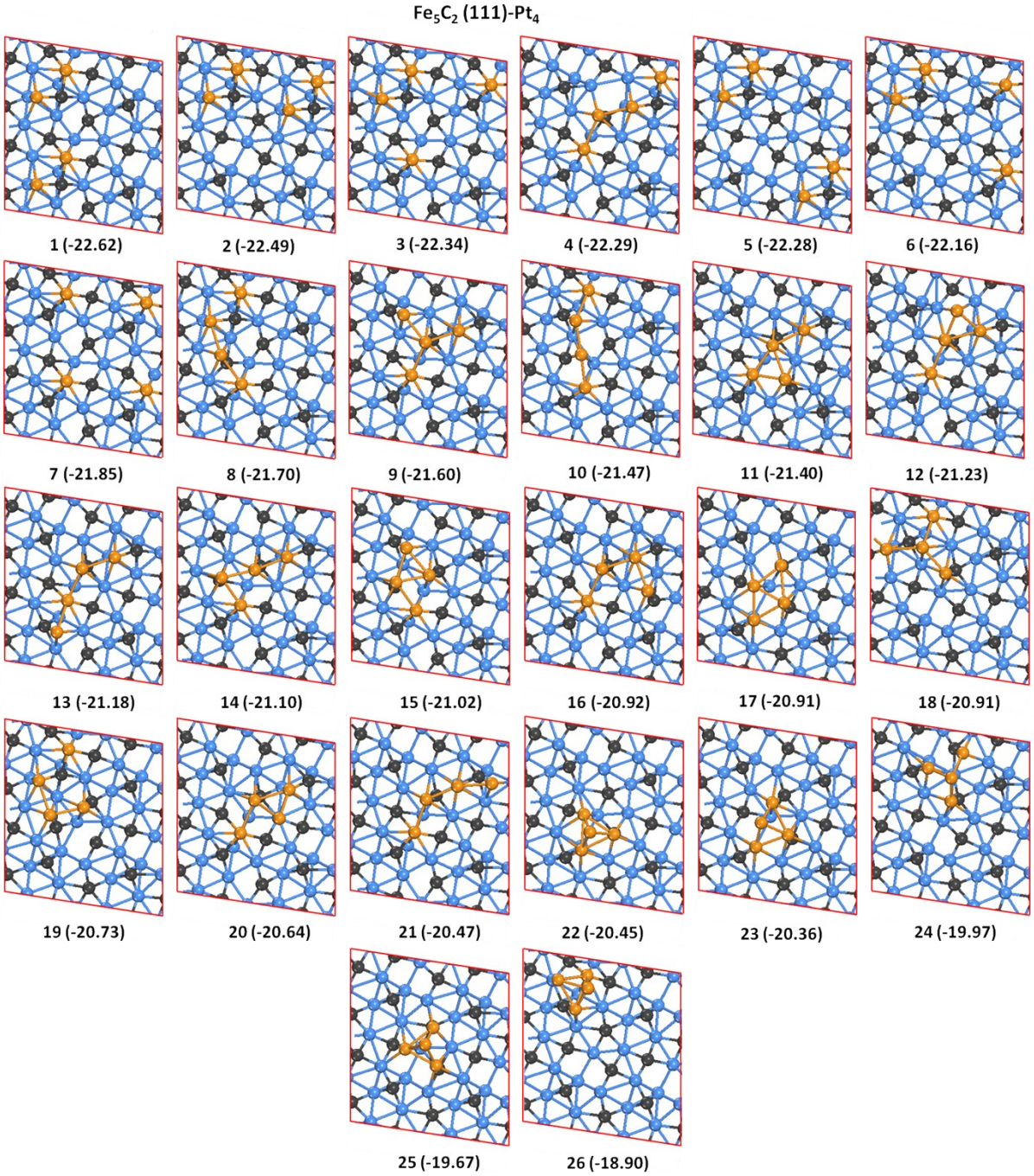

Figure S8. Various structures and adsorption energies for Pt_4 on the Fe_5C_2 (111) surface (adsorption energy in eV)

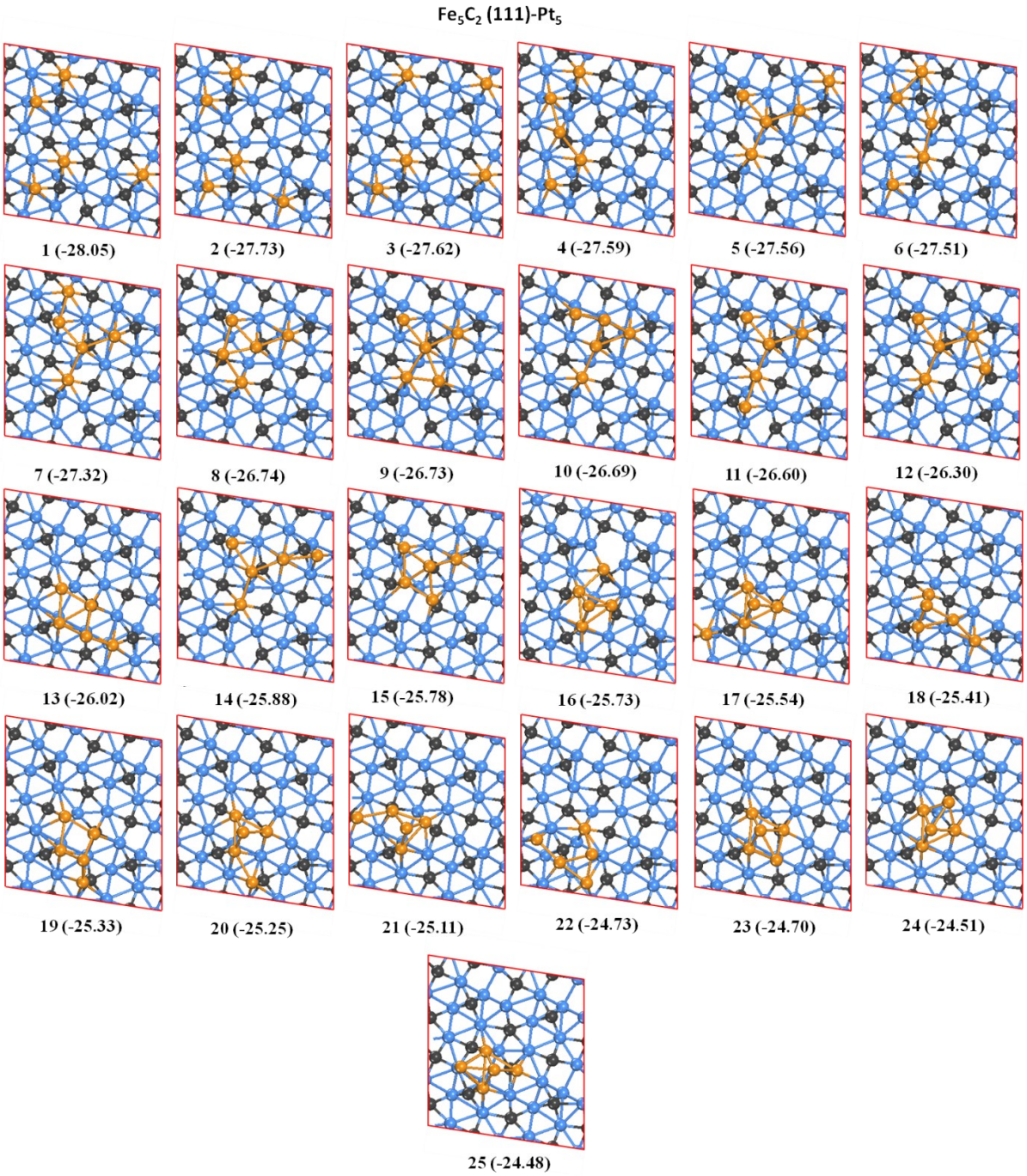

Figure S9. Various structures and adsorption energies for Pt_5 on the Fe_5C_2 (111) surface (adsorption energy in eV)

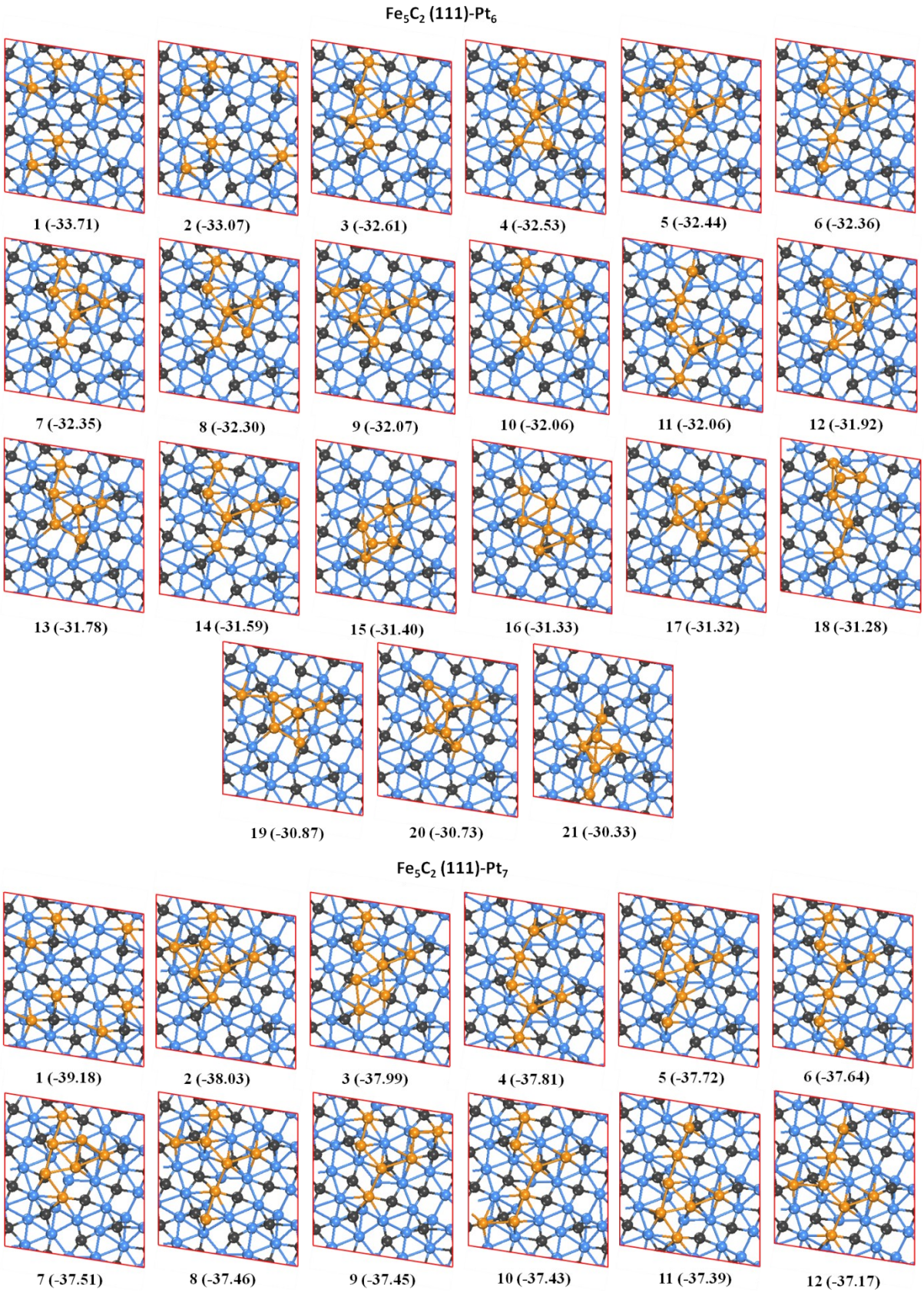

Figure S10. Various structures and adsorption energies for Pt_n (n = 6, 7) on the Fe_5C_2 (111) surface (adsorption energy in eV)

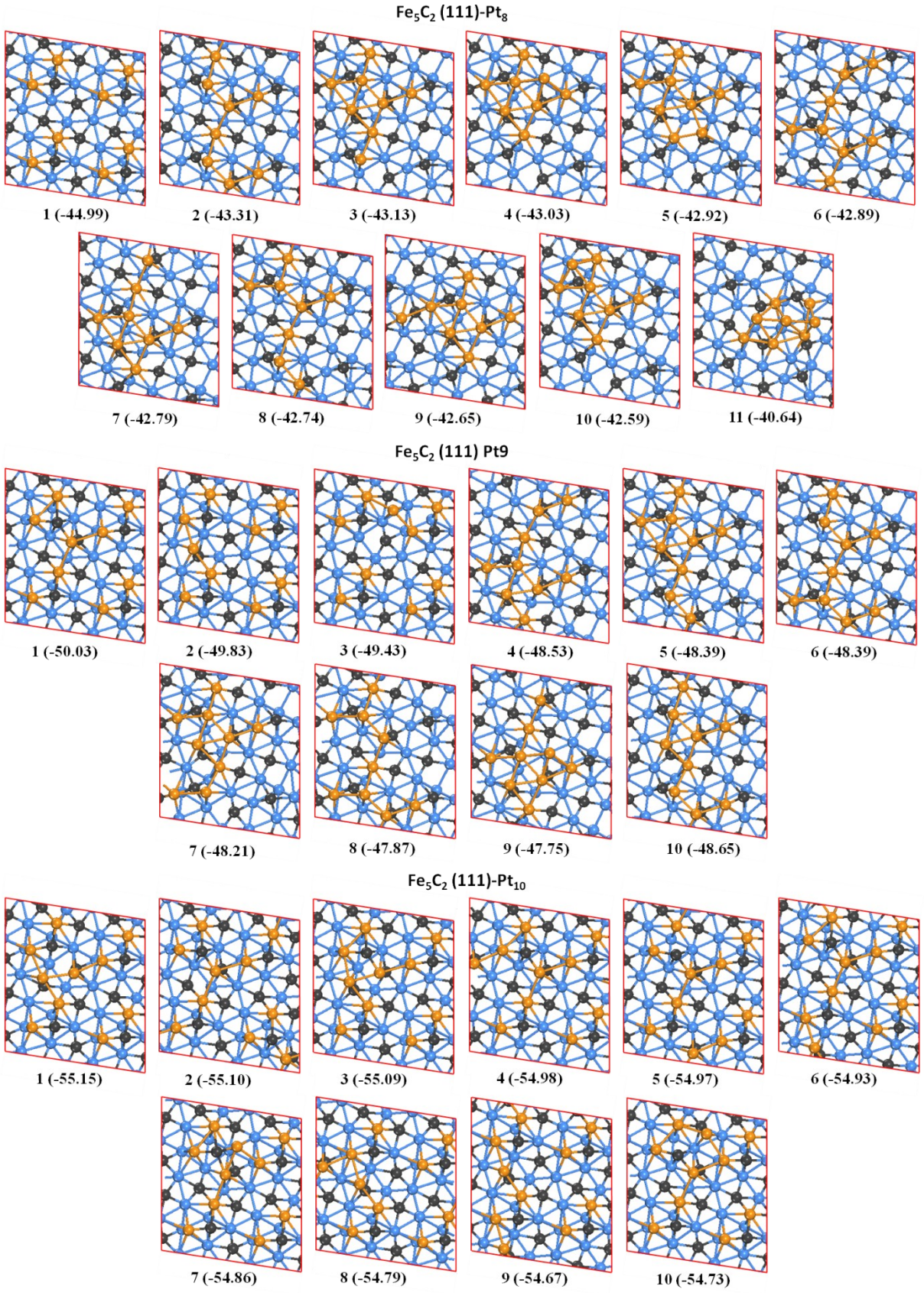

Figure S11. Various structures and adsorption energies for Pt_n (n = 8–10) on the Fe_5C_2 (111) surface (adsorption energy in eV)

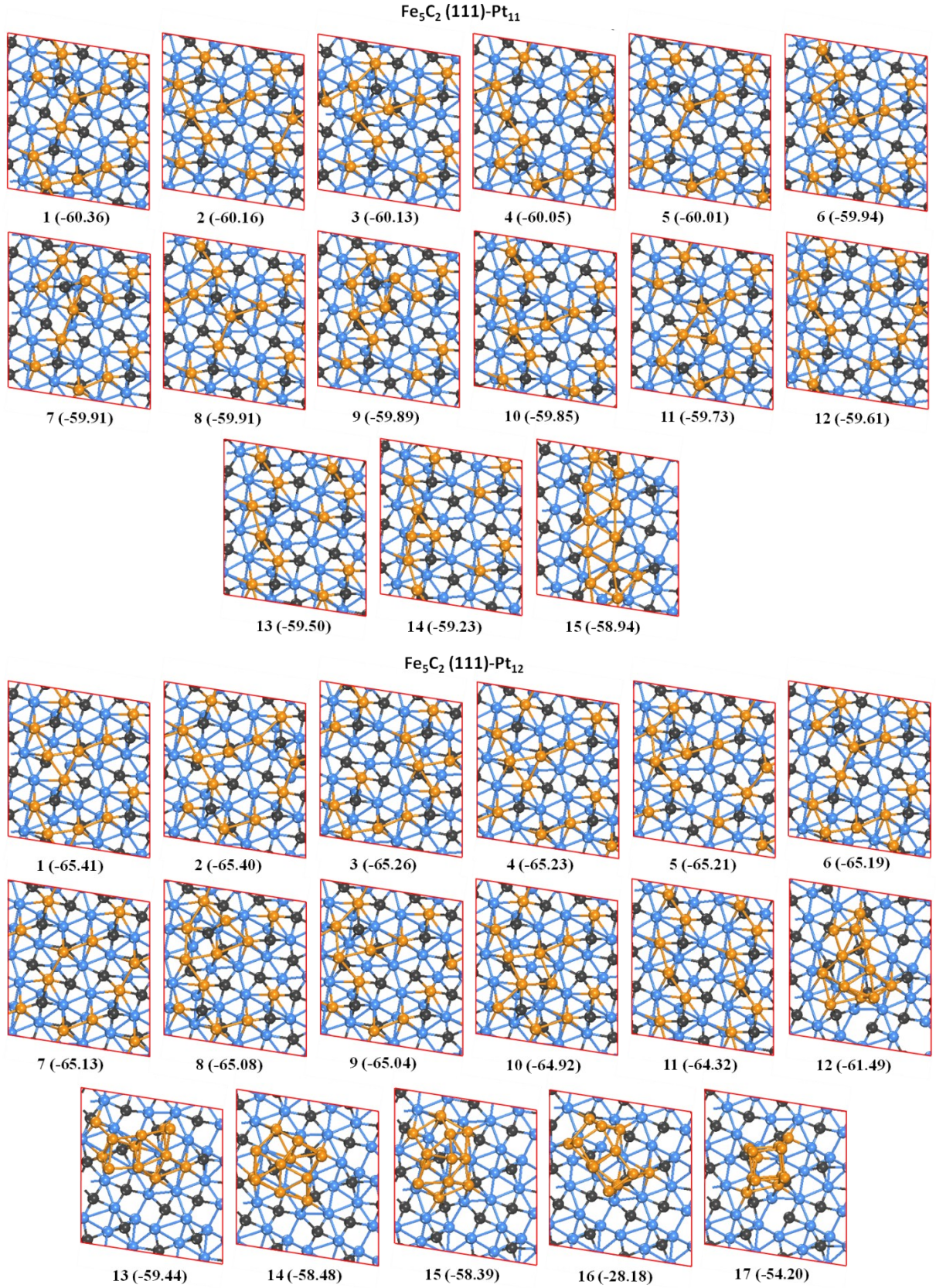

Figure S12. Various structures and adsorption energies for Pt_n (n =11, 12) on the Fe_5C_2 (111) surface (adsorption energy in eV)

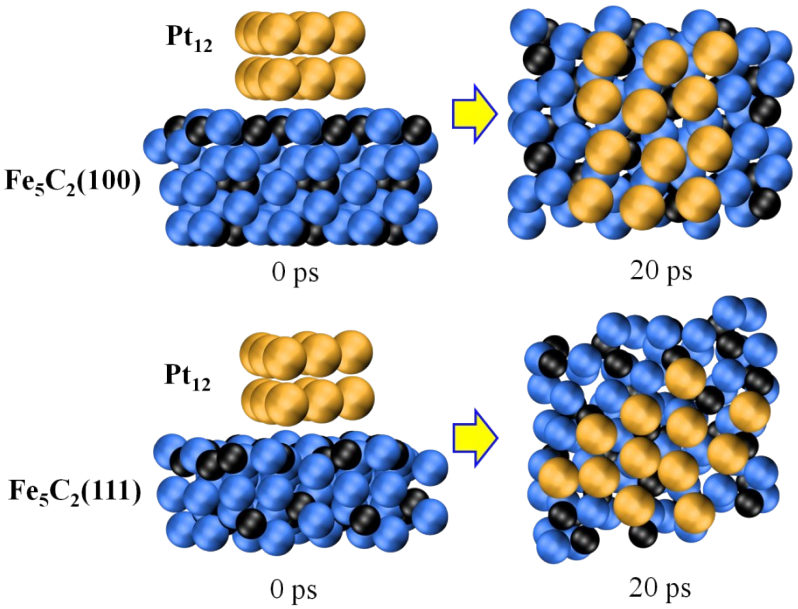

Fig. S13 The snapshot of initial and final structures at 20ps in AIMD calculation of Pt_{12} cluster deposited on the $Fe_5C_2(100)$ and (111) surfaces. The Pt atoms are in orange, the Fe atoms in blue and the C atoms in black.

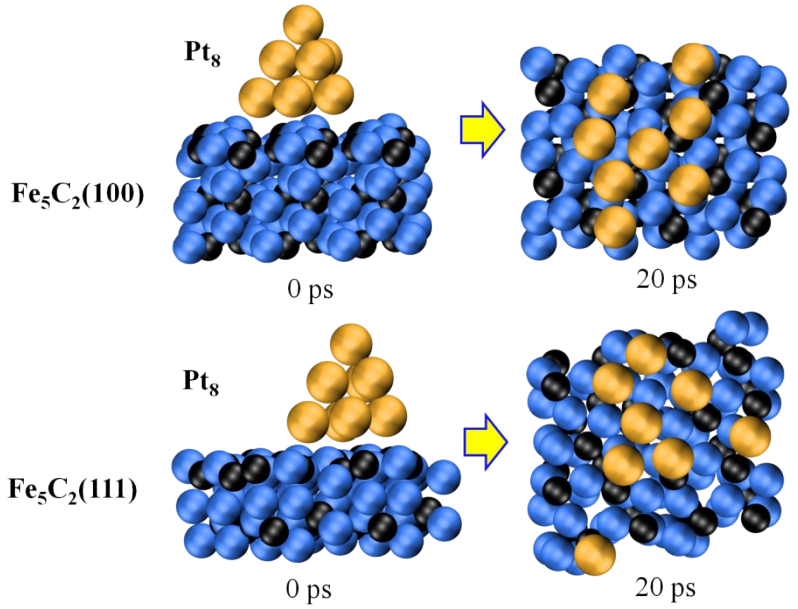

Fig. S14 The snapshot of initial and final structures at 20ps in AIMD calculation of Pt_8 cluster deposited on the $Fe_5C_2(100)$ and (111) surfaces. The Pt atoms are in orange, the Fe atoms in blue and the C atoms in black.