Computational Study of Pt-Zn Clusters on Stoichiometric MgO(100) and TiO₂(110): Dramatically Different Sintering Behavior

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Supporting Information

		Pt ₃ Zn			Pt ₂ Zn ₂		
		Rhom-C ₅	Tetr-C ₁		Rhom-C ₅ /C _{2H}	Sqrpln-C _{2V}	
		M=1	M=1	M=3	M=1	M=1	M=3
B3LYP	LANL2DZ	-2.11	-2.00	-2.07	-1.64	-1.67	-1.52
	GEN	-2.04	-1.92		-1.57	-1.59	
	PBE	-4.20			-3.11	-3.09	
	MP2	-4.38			-3.32		
		Pt ₂ Zn ₂		PtZn ₃		Zn ₄	
		Tetr-C ₁		Trgpln-C ₁	Rhom-C ₅ /C _{2H}	Tetr- C ₁	Rhom- C ₁
		M=1	M=3	M=1	M=1	M=1	M=1
B3LYP	LANL2DZ	-1.40	-1.43	-1.04	-0.82	-0.03	-0.03
	GEN	-1.36	-1.37	-0.97	-0.81	-0.06	-0.06
	PBE	-2.88	-2.89	-1.77	-1.66	-0.26	
	MP2		-2.89	-1.82	-1.71	-0.24	

Table S1. Gaussian results for listed gas-phase clusters. Binding energies per atom are in eV, global minima are in bold. The structure and multiplicity of the cluster are shown. GEN is the large basis set shown in the text. Results show good agreement with Quantum Espresso, pseudo-gas-phase, results.

Figure S1. By scaling the given empirical chemical potentials for Zn, the evaporation & redeposition rates can be adjusted such that their respective crossings are brought within the total range of adsorption energies experienced by the Zn monomer on both the MgO and TiO_2 supports.

Figure S2. Projected-Density of States on both the MgO (a—d) and TiO₂ (e—h) supports; for Pt₄ (a,e), Pt₂Zn₂ (b,c,f,g), and Zn₄ (d,h) clusters. Zn₄ on TiO₂ does show that some of the PDOS is brought nearer the Fermi energy, with some hybridization between O's *S* and *P* projections with Zn's *S*-wave.

Figure S3. Intra-cluster Coulomb interaction for the various tetramers on MgO (red) and TiO₂ (blue) supports. Electrostatic potential energy is a minimum for the Pt₂Zn₂ clusters on either support.