Supporting Information of:

DFT study of the structure, chemical ordering and molecular adsorption of Pd-Ir nanoalloys

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Table 1. Detailed comparison of the lattice constant, cohesive energy, and bulk modulus for bulk Pd (fcc) and Ir (fcc) with experimental and theoretical data.

		This method	Reference (PBE)	Experiment
Lattice parameter	Pd	3.940	3.95[3]	3.88[1]
(Å)	Ir	3.872	3.89[5]	3.84[6]
Cohesive energy	Pd	3.743	3.63[3]	3.89[2]
(eV/atom)	Ir	7.351	8.96[5]	6.94[2]
Bulk modulu	Pd	168.96	166[4]	181[2]
(GPa)	Ir	345.78	340[5]	355[7]

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