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Structural Investigation of the Ternary PdRuM (M=Pt, Rh, or Ir) Nanoparticles Using First-Principles Calculations

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1 Additional Figures and Tables

Table S 1: Formation energy of pure NPs in three shapes. The formation energy of the Pd NP in tOh_{55} shape is missing. Since the particular NP is unstable and transforms into the Ih shape.

	E_f (eV/atom)				
	Pd	Ru	Pt	Rh	Ir
hcp_{57}	0.91	1.57	1.06	1.29	1.58
tOh_{55}	–	1.64	1.09	1.31	1.63
Ih_{55}	0.91	1.61	1.6	1.28	1.59

Table S 2: Comparison of oxygen adsorption energies between fcc (111) and hcp (10$\bar{1}$1) surfaces. The adsorption sites are both on 3-fold fcc site.

	E_{ads} (eV/atom)				
	Pd	Ru	Pt	Rh	Ir
3-fold fcc site on fcc (111) surface	-1.93	-3.21	-1.81	-2.68	-2.65
3-fold fcc site on hcp (10$\bar{1}$1) surface	-2.06	-3.65	-1.84	-2.78	-2.47

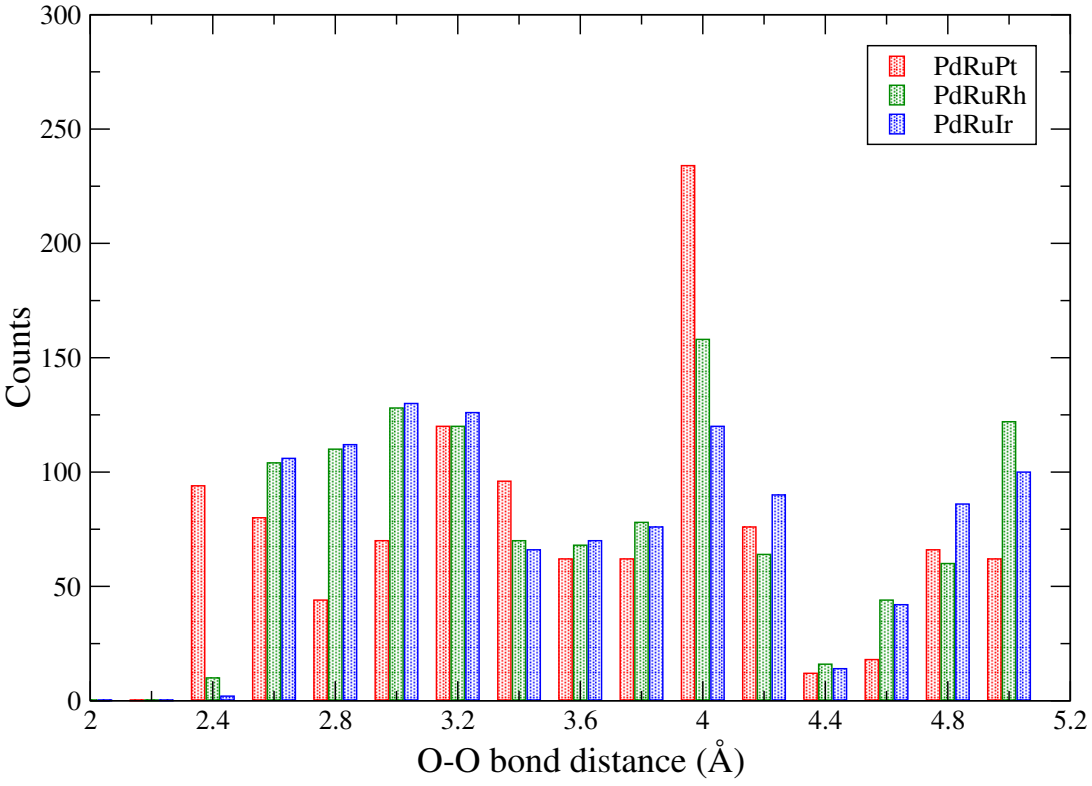

Figure S 1: The O-O bond length distribution with regard to oxidized ternary PdRuPt, PdRuRh, and PdRuIr NPs. The statistic of individual ternary NP includes NPs with hcp, tOh and Ih shapes.