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Towards stable single-atom catalysts: Strong binding of atomically dispersed transition metals on the surface of nanostructured ceria

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Supporting Information

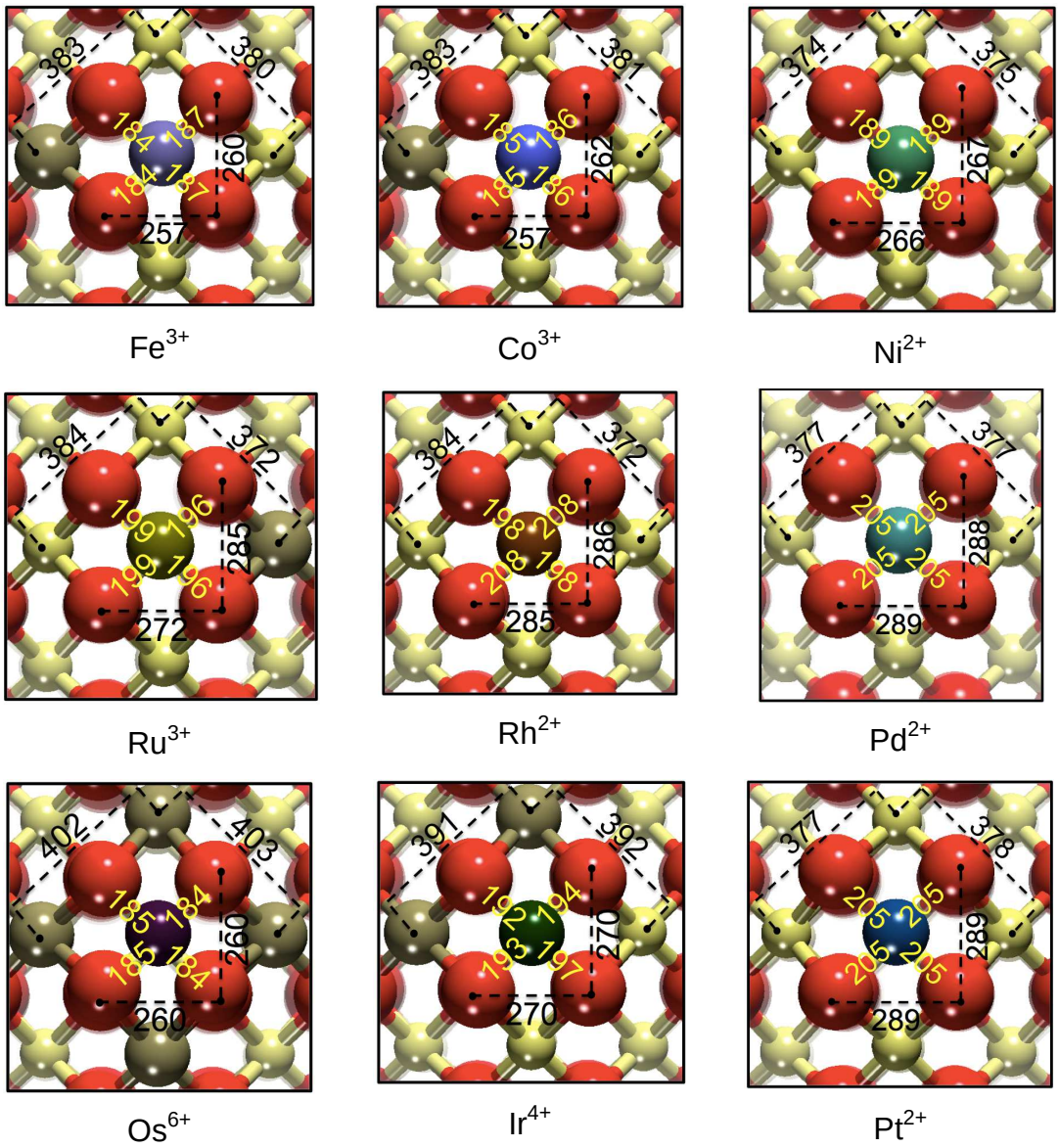

Figure S1. Representative M-O, O-O and Ce-Ce distances (in pm) at the {100} facet of the $Ce_{40}O_{80}$ NP with adsorbed metal atoms (M) of Groups VIII, IX and X of the Periodic Table.

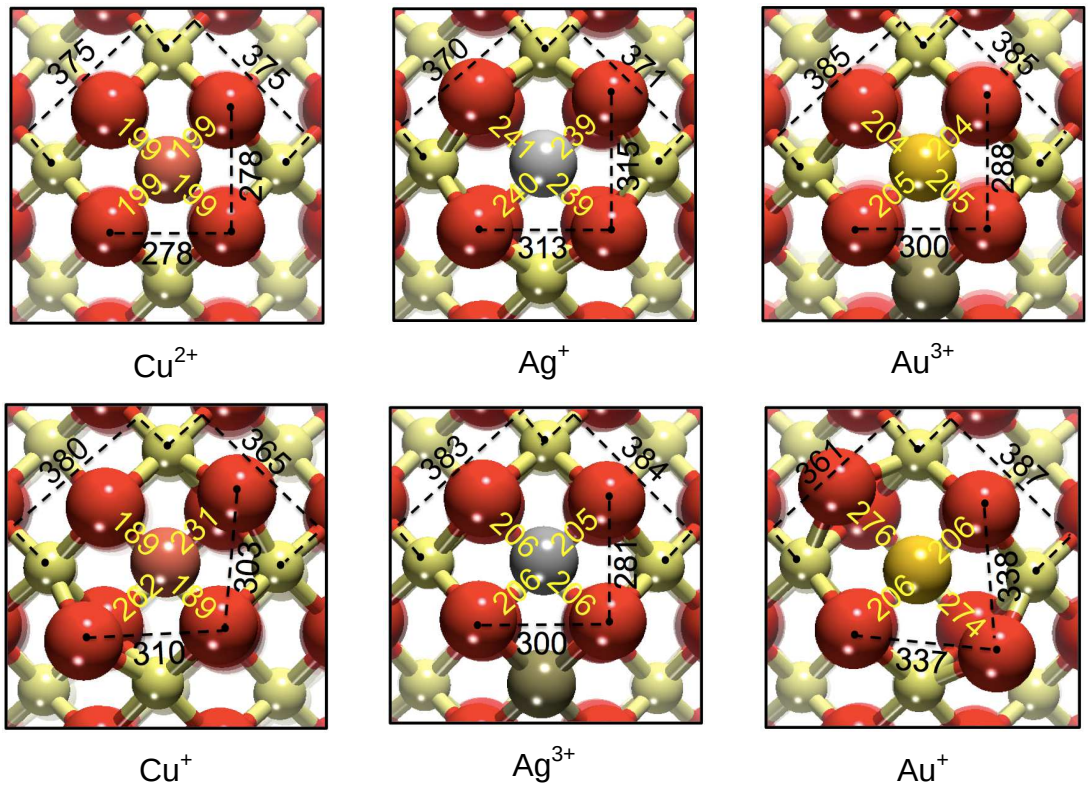

Figure S2. Representative M-O, O-O and Ce-Ce distances (in pm) at the {100} facet of the $Ce_{40}O_{80}$ NP with adsorbed metal atoms M = Cu, Ag, Au atoms in two possible oxidation states. The panels in the upper row correspond to the most stable calculated states.

Table S1. Experimental cohesive energies (in kJ/mol) of transition metals.[a]

Group VIII		Group IX		Group X		Group XI	
-413	Fe	-424	Co	-428	Ni	-336	Cu
-650	Ru	-554	Rh	-376	Pd	-284	Ag
-788	Os	-670	Ir	-564	Pt	-368	Au

[a] C. Kittel, *Introduction to Solid State Physics*. 8th Ed., Hoboken, NJ: J. Wiley, 2005, 50.

Table S2. Experimental standard heats of formation $\Delta_f H$ (in kJ/mol) of the most stable oxides of the metals (M) studied in the present work.[a,b]

Group VIII		Group IX		Group X		Group XI	
-825.5	Fe_2O_3	-237.5	CoO	-244.3	NiO	-175.3	CuO
-314.8	RuO_2	-405.5	Rh_2O_3	-118.6	PdO	-29.0	Ag_2O
-291.8	OsO_2	-249.5	IrO_2	-80.0	PtO	-13.0	Au_2O_3

[a] M. W. Chase, *NIST-JANAF Thermochemical Tables*. 4rd Ed., Journal of Physical and Chemical Reference Data, 1998.
[b] O. Kubaschewski, C. B. Alcock, *Metallurgical Thermochemistry*. 5th Ed., Pergamon Press, 1983.