

The degradation of transition metal@Pt core-shell nanoparticle catalyst: A DFT study

Lu Li^{1,2}, Hong xin Ma^{1,3}, Xiao dong Jian⁴, Ping Qian^{1,2*}, Yan jing
Su^{1,3*}

¹ Beijing Advanced Innovation Center for Materials Genome Engineering, University of
Science and Technology Beijing, Beijing, China

² Department of Physics, University of Science and Technology Beijing, Beijing, China

³ Corrosion and Protection Center, University of Science and Technology Beijing, Beijing,
China

⁴ National Supercomputer Center in Tianjin, Tianjin, China

Supplementary Information

Table S1. Spin states of ICO structure M@Pt core-shell nanoparticles. M_{Pt} represents the average spin moments of Pt atoms, M_c represents the average spin moments of core atoms, M_t represents the total spin moments of M@Pt nanoparticles, and N represents the total number of atoms in M@Pt nanoparticles.

	M_{Pt} (μ_B /atom)	M_c (μ_B /atom)	M_t (μ_B)	N
Fe@Pt	0.24	2.94	183.78	147
Co@Pt	0.19	1.89	121.43	147
Ni@Pt	0.17	0.86	62.94	147
Cu@Pt	0	0	0	147
Ru@Pt	0	0	0	147
Rh@Pt	0	0	0	147
Pd@Pt	0.25	0.53	52.15	147
Ag@Pt	0	0	0	147
Os@Pt	0	0	0	147
Ir@Pt	0	0	0	147
Pt@Pt	0	0	0	147
Au@Pt	0	0	0	147

Table S2. Spin states of Cubo structure M@Pt core-shell nanoparticles. M_{Pt} represents the average spin moments of Pt atoms, M_c represents the average spin moments of core atoms, M_t represents the total spin moments of M@Pt nanoparticles, and N represents the total number of atoms in M@Pt nanoparticles.

	M_{Pt} (μ_B /atom)	M_c (μ_B /atom)	M_t (μ_B)	N
Fe@Pt	0.25	2.82	178.10	147
Co@Pt	0.17	1.89	119.59	147
Ni@Pt	0.16	0.77	57.07	147
Cu@Pt	0	0	0	147
Ru@Pt	0	0	0	147
Rh@Pt	0	0	0	147
Pd@Pt	0.26	0.43	47.57	147
Ag@Pt	0	0	0	147
Os@Pt	0	0	0	147
Ir@Pt	0	0	0	147
Pt@Pt	0	0	0	147
Au@Pt	0	0	0	147

Table S3. Spin states of TCO structure M@Pt core-shell nanoparticles. M_{Pt} represents the average spin moments of Pt atoms, M_c represents the average spin moments of core atoms, M_t represents the total spin moments of M@Pt nanoparticles, and N represents the total number of atoms in M@Pt nanoparticles.

	M_{Pt} (μ_B /atom)	M_c (μ_B /atom)	M_t (μ_B)	N
Fe@Pt	0.21	2.84	249.98	201
Co@Pt	0.13	1.85	162.01	201
Ni@Pt	0.13	0.81	79.85	201
Cu@Pt	0	0	0	201
Ru@Pt	0	0	0	201
Rh@Pt	0	0	0	201
Pd@Pt	0.06	0.16	19.96	201
Ag@Pt	0	0	0	201
Os@Pt	0	0	0	201
Ir@Pt	0	0	0	201
Pt@Pt	0	0	0	201
Au@Pt	0	0	0	201

The specific coordinates of the optimized core-shell nanoparticle models

POSCAR of ICO-structure Ir@Pt core-shell nanoparticle

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0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000
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POSCAR of Cubo-structure Ir@Pt core-shell nanoparticle

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