

Supporting Information

A Comprehensive Understanding of the Melting Temperature of Nanocrystals:

Implications for Catalysis

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Table S1. The parameters required for calculation.

	h (nm) ¹	H_m (kJ/mol) ¹	T_m (K) ¹	S_{vib} (J/mol K) ²	V_s (cm ³ /mol) ¹
Sn	0.372	-	-	9.22	-
Bi	0.407	-	-	7.20	-
Au	0.319	-	-	7.62	-
Ni	0.249	17.20	1728.00	8.11	6.59
Al	0.316	10.79	933.25	6.15	10.00
In	0.386	3.26	429.76	7.59	15.70
Ag	0.319	11.30	1234.00	7.82	10.27
Pd	0.275	-	-	7.22	-
Pt	0.278	-	-	7.82	-

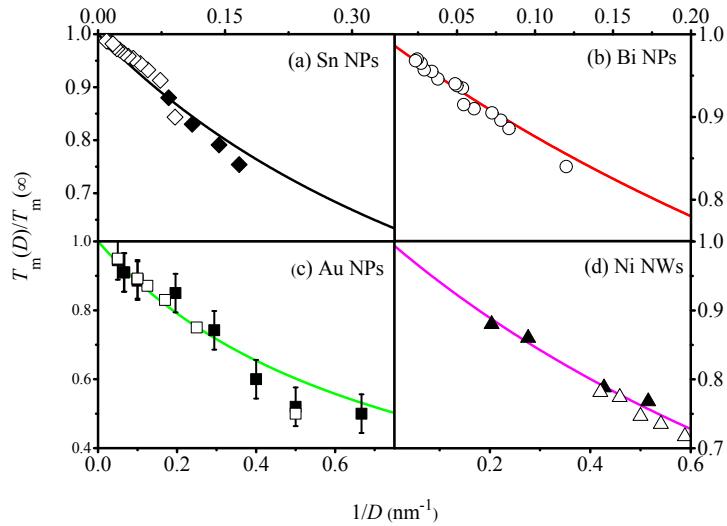


Fig. S1. The calculated $T_m(D)$ according to Eq. (7) for (a) Sn NPs, (b) Bi NPs, (c) Au NPs and (d) Ni NWs, respectively. The symbols rhombs (\diamond^3 and \blacklozenge^4), circles (\circ^5), squares (\blacksquare^6 and \square^7), triangles (\blacktriangle^8 and \triangle^9) are corresponding experimental results.

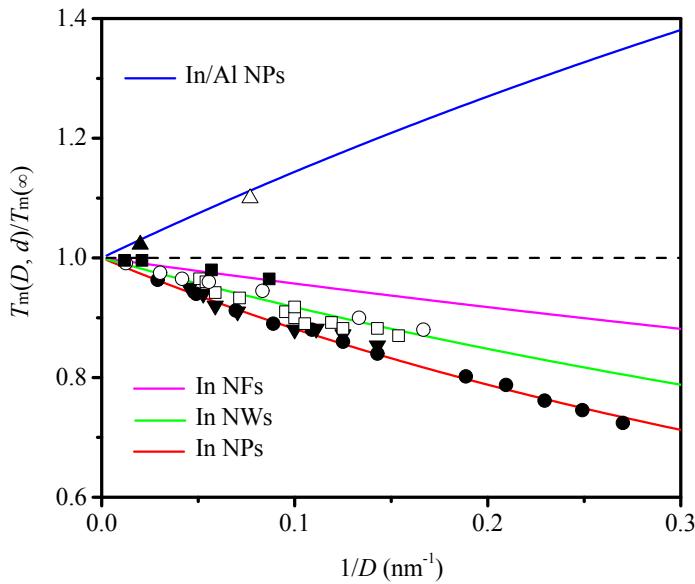


Fig. S2. $T_m(D, d)$ of In NCs as functions of D and d under different interface conditions. The blue line is the calculated results according to Eq. (9) for In/Al NPs and the symbols Δ^{10} and \blacktriangle^{11} denote experimental data. The pink, black and red lines represent $T_m(D, d)$ according to Eq. (7) for In NFs, NWs and NPs, respectively. The symbols \bullet^{12} , \blacktriangledown^{13} , \circ^{14} , \square^5 and \blacksquare^{15} are experimental results for In NPs, NWs and NFs.

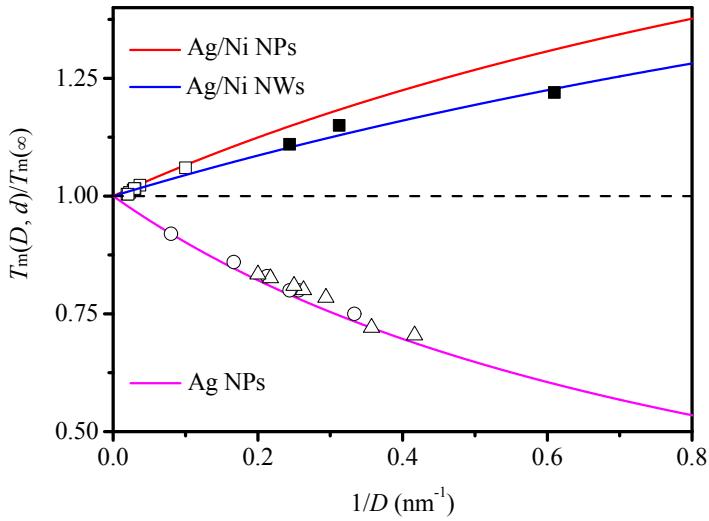


Fig. S3. $T_m(D, d)$ of Ag NCs as functions of D and d under different interface conditions. The red and blue lines are the calculated results according to Eq. (9) for Ag/Ni NPs and NWs. The symbols \bullet^{16} and \blacksquare^{17} are the corresponding experimental and simulation results. The black line represents $T_m(D)$ according to Eq. (7) for Ag NPs and the symbols Δ^{18} and \circ^{19} are the simulation data.

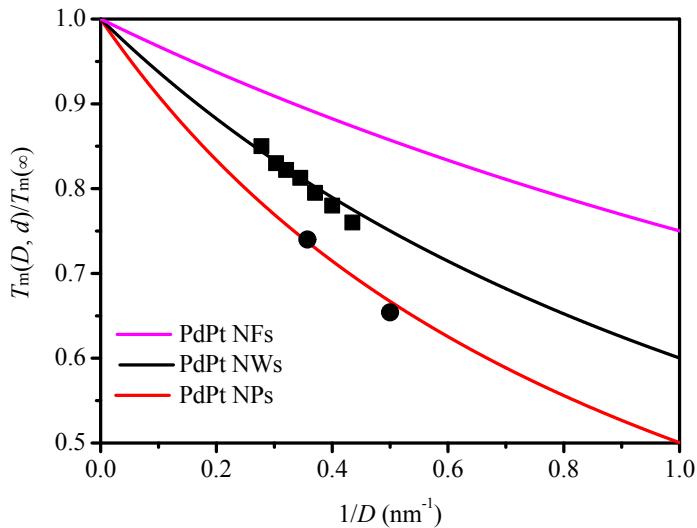


Fig. S4. $T_m(D, d)$ of $Pd_{0.5}Pt_{0.5}$ NCs as functions of D and d according to Eq. (11). From the top down, the pink, black and red lines represent $T_m(x, D, d)$ for NFs, NWs and NPs, respectively. The symbols \bullet^{20} and \blacksquare^{21} are the simulation results for NPs and NWs, respectively.

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