

Electronic Supplementary Information

Well-faceted noble-metal nanocrystals with nonconvex polyhedral shapes






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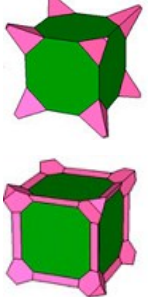

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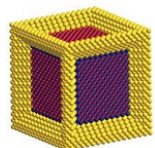
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Table 1 Summary of typical cases of NCs with nonconvex polyhedral structures synthesized using capping agents.





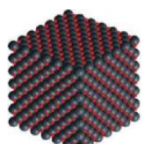

Morphologies	Ideal Exposed Facets	Metals	Capping agents	Metal Precursors	Other reactants and/or solvent	Methods, temperature and reaction time	Reference
	{110}	PtCu ₃	<i>N</i> -butylamine CTAC	Pt(acac) ₂ Cu(acac) ₂	DMF	Solvothermal synthesis, 150 °C for 10 h	26
	{411}	Pt	Methylamine PVP	H ₂ PtCl ₆	DMF	Solvothermal synthesis, 160 °C for 11 h	35
	{211}	Pt	1-octylamine	Pt(acac) ₂	1-octylamine	Solvothermal synthesis, 200 °C for 3 h	36
	{720}	Au	CTAC in presence of Ag ⁺ ions	Au seeds HAuCl ₄	AA HCl H ₂ O	Seeded growth, ambient temperature	40
	{110}+{100}	Pd	CTAB in presence of Cu ²⁺ ions	Pd seeds H ₂ PdCl ₄	AA H ₂ O	Seeded growth, 40 °C for 12 h	70

	{hhl}	Au	CTAC	Au seeds HAuCl ₄	AA H ₂ O	Seeded growth, 25 °C for 1 h	69
	{110}	Au	CTAC	HAuCl ₄	AA H ₂ O	One-step synthesis, 4–6 °C , 8 h	68
	{110}	Au-Pd	CTAC	HAuCl ₄ H ₂ PdCl ₄	AA H ₂ O	One-step synthesis, 20 °C for 2 min and then cooled down to 6 °C, 8 h	68
	/	Pd	KBr, PVP	Pd seeds Na ₂ PdCl ₄	H ₂ O	Seeded growth, low temperature or low injection rate	89
	{110}	Rh	PVP	Na ₃ RhCl ₆	AA CA TriEG	Injecting precursors to the preheated reactants and then keep at 145 °C for 3 h	67

	/	Rh-Pd	PVP, KBr	Pd seeds Na_3RhCl_6	EG	Seeded growth, injecting Rh precursors to the preheated reactants and then stay at 140 °C for 10 min	90
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Notes: DMF = *N, N*- dimethyl formamide; PVP = poly(vinyl pyrrolidone); AA = *L*-ascorbic acid; CTAC = cetyltrimethylammonium chloride; CTAB = cetyltrimethylammonium bromide; TriEG = triethylene glycol; CA = citric acid; EG = ethylene glycol.

Table 2 Summary of typical cases of NCs with nonconvex polyhedral structures from etchants mediated synthesis.

Initial shapes	Final shapes	Metals	Etchants and etching mechanism	Solvent	Temperature	Reference
		Ag	Using $\text{NH}_4\text{OH}/\text{H}_2\text{O}_2$ to etch away Ag atoms	A solution of PVP and water	4 °C	91
		Pt-Ni alloy	Using the coordination of Ni with dimethylglyoxime to etch away Ni atoms	Water and ethanol	Room temperature	92
		Pd	Galvanic replacement Pd with H_2PtCl_6 to etch away Pd atoms	Aqueous solution containing PVP and KBr	90 °C	93





		Pd	Making use of the gradients of surface energy caused by heating the reverse micelle to etch away Pd atoms	Reverse micelle made of CTAB/octanol/H ₂ O	105 °C	94
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Table 3 Summary of typical cases of NCs with nonconvex polyhedral structures from templates directed overgrowth and etching synthesis.

Nanocages	Metals	Facets	Templates	Overgrowth condition, temperature and time	Etching condition, temperature and time	Reference
	Pt	{100}	Cubic Pd	Na ₂ PtCl ₆ solution in EG were injected into the preheated EG solvent containing Pd seeds, AA, KBr, and PVP with 4.0 mL/h, and then stay at 200 °C for another 1 h	Etching in an aqueous solution containing FeCl ₃ , KBr, PVP and HCl and stay at 100 °C for 3 h	28
	Pt	{111}	Octahedral Pd		Etching in an aqueous solution containing FeCl ₃ , KBr, PVP and HCl and stay at 100 °C for 4 h	