Tuning Structure of Bimetallic Nanoparticles In Catalysis Applications

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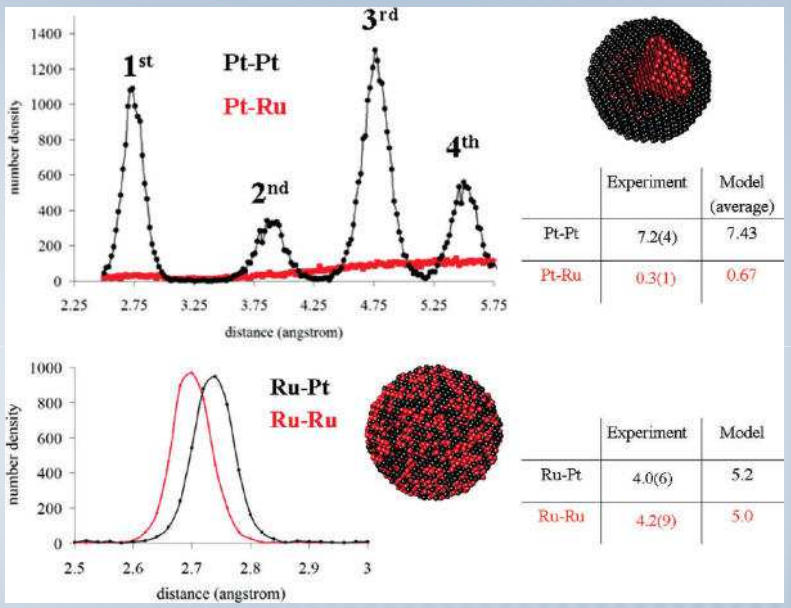
- Bimetallic heterogeneous catalysts has been widely applied in catalysis science: fuel cells, catalytic reforming and hydrogenation, for instance. The ability to control the composition, shape and architecture of these bimetallic systems are of importance in tailoring the propertied and catalytic activities.

- Core-shell (Ru@Pt) and alloyed PtRu bimetallic nanoparticles with similar compositions and particle sizes (~ 4.0 nm) were synthesized and subjected to a comprehensive structural characterization using XAFS, XRD/PDF and TEM-EDS. The studies show clear pictures of two types of NP architectures in the core-shell and alloyed NPs. While XRD and TEM-EDS afford the general information that differentiates the core-shell from the alloy NP types, EXAFS and PDF analyses provide detailed and spatially resolved structural information regarding the core / shell interfaces and local bonding environments. The 4.4 nm PtRu (1:1) alloys are crystalline homogeneous random alloy; while 4.0 nm Ru@Pt NPs have 1 - 2 monolayer of thick Pt crystalline shells sit on top of the highly distorted hcp Ru cores.

- Evidence shows that different architectures impart marked difference in chemical and catalytic activities. A combination of various characterization analyses can provide complementary information used to construct a detailed structural pictures; which is critical to understand the properties and catalytic chemistry. Such information provides theoretical evidence for tuning the structure of bimetallic nanoparticles for applications in specific catalytic reactions.



	Experiment	Model (average)
Pt-Pt	7.2(4)	7.43
Pt-Ru	0.3(1)	0.67

	Experiment	Model
Ru-Pt	4.0(6)	5.2
Ru-Ru	4.2(9)	5.0

Plots of pair distributions predicted from model Ru@Pt core-shell structures with a 2.0 ML Pt shell (top) and PtRu (1:1) alloys (bottom). The table insets show the calculated and observed EXAFS derived partial coordination numbers of the two NP architectures.

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Work performed on beamlines X18B.