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An experimental and computational investigation of structural dependence of catalytic properties of Pt-Ru nanoparticles[1] BINAY PRASAI, Central Michigan University — An approach to determining the 3D atomic structure of metallic nanoparticles (NPs) in fine detail is described and exemplified on Pt–Ru alloy NPs of importance to the development of devices for clean energy conversion such as fuel cells. NPs are characterized structurally by total scattering experiments involving high-energy synchrotron X-ray diffraction coupled to atomic pair distribution functions (PDFs) analysis. 3D structure models are built by molecular dynamics simulations and further refined against the experimental PDF data by reverse Monte Carlo simulations and analyzed in terms of structural characteristics. Structural characteristics of activated NPs and data for their catalytic activity are compared side by side and strong evidence found that electronic effects, indicated by significant changes in Pt–Pt and Ru–Ru metal bond lengths at NP surface, and practically unrecognized so far atomic ensemble effects, indicated by distinct stacking of atomic layers near NP surface and prevalence of particular configurations of Pt and Ru atoms in these layers, contribute to the observed enhancement of the catalytic activity of PtxRu100−x alloy NPs at x $\sim$ 50.

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