

# **Combined Experimental and Theoretical Investigation of Formation of Pt(111) Nanoparticle Layers Grown on Ru(0001) Core**

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To achieve direct methanol fuel cell technology commercially viable, the principle drawbacks, namely high Pt-loadings in anode and cathodes, the sluggish kinetics of the anodic methanol oxidation reaction needs to be addressed. Several important investigations on design and development of electrode configurations to solve these issues have shown that the reaction kinetics of MOR depend strongly on the surface structure, size, amount, dispersion of the catalyst nanoparticles, and the nature of the support material. For fully understanding the functional effect of these controlling parameters on the electrochemical reactions, the relation amongst these structural features and the corresponding reaction kinetics are necessary, the results of which can then be connected with theoretical considerations for deeper understanding to further improving the catalyst performance. This lecture presents our recent works on systematic experimental HRTEM measurements combined with density functional theory (DFT) computational approach employed for investigating the relations of Pt-Ru bimetallic nanoparticles. A layer growth mechanism of Pt-Ru bimetallic nanoparticles has been proposed with supporting experiments and calculations by density functional theory. Elongated Pt atoms on Ru nanoparticles were synthesized via a two step route, and their structural details were obtained by high-resolution transmission electron microscopy. Because of the intrinsic mismatch of lattice spacing between the two elements, such an unusual growth was analyzed with the DFT simulations to explore the mystery of the growth mechanism. Pt atoms would rearrange the packing order and adjust the Pt-Pt atomic distance, and so do the Ru nanoparticles in order to achieve the optimal energy status of the bimetallic system. The resultant Pt(111) layers could stack on top of the Ru(0001) core more tightly by fitting the pockets left between the Ru atoms. The findings give insight into the formation mechanism of the nanosized Pt-Ru bimetallic catalyst and pave the way for designing bimetallic catalysts with tailored properties at the atomic level.

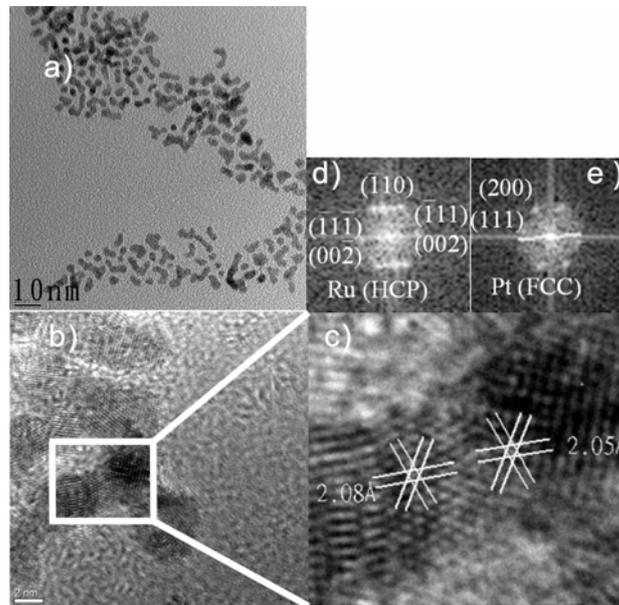


FIG. 1. (a) HRTEM image of Pt-on-Ru NPs. (b)-(c) Domain of single particle of Ru(0001) and Pt(111) in a small scale. (d) Fourier transform pattern for Ru region. (e) Fourier transfer pattern for Pt region.

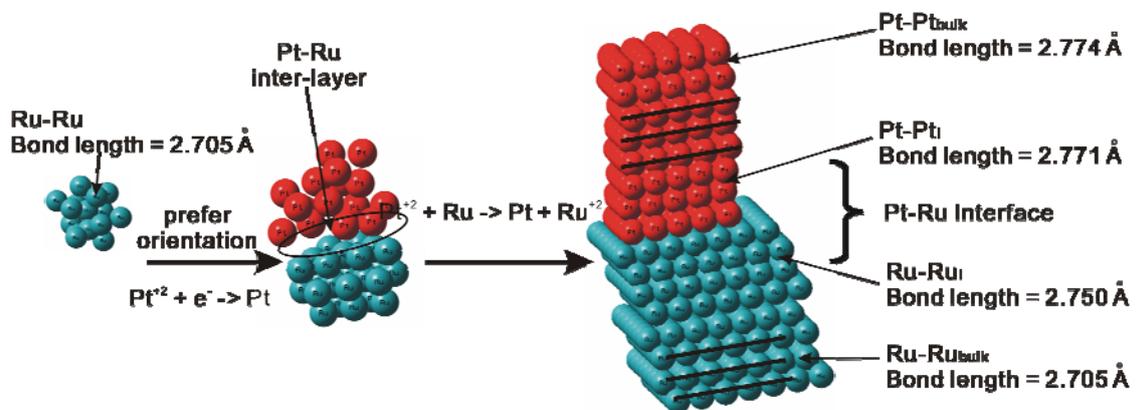


FIG. 2. Illustrative formation of core-shell structured elongated PtRu NPs accounting for experimental and DFT simulation.