Supplementary Information

Trimetallic nanostructures: the case of AgPd/Pt multiply twinned nanoparticles

Subarna Khanal,[†] Nabraj Bhattarai,[†] J. Jesus Velazquez-Salazar,[†] Daniel Bahena,[†] German Soldano,[§] Arturo Ponce,[†] Marcelo M. Mariscal,[§] Sergio Javier Mejia-Rosales,[‡] and Miguel Jose-Yacaman[†]*

[†]*Department of Physics and Astronomy, University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249, United States*

[§]*INFIQC/CONICET, Departamento de Matematica y Fisica, Facultad de Ciencias Quimicas, Universidad Nacional de Cordoba, XUA5000 Cordoba, Argentina*

[‡]*Center for Innovation and Research in Engineering and Technology, and CICFIM-Facultad de Ciencias Fisico-Matematicas, Universidad Autonoma de Nuevo Leon, San Nicolas de los Garza, NL 66450, Mexico*

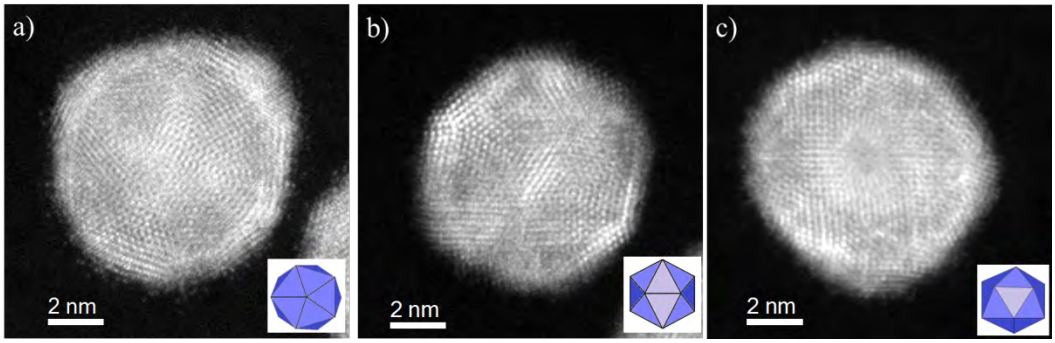

Fig. S1 High magnification of HAADF images of icosahedral structure along (a) 5-fold, (b) 2-fold, and (c) 3-fold symmetry axis and the insets shows corresponding schematic diagram of the icosahedral structure different symmetry axes.

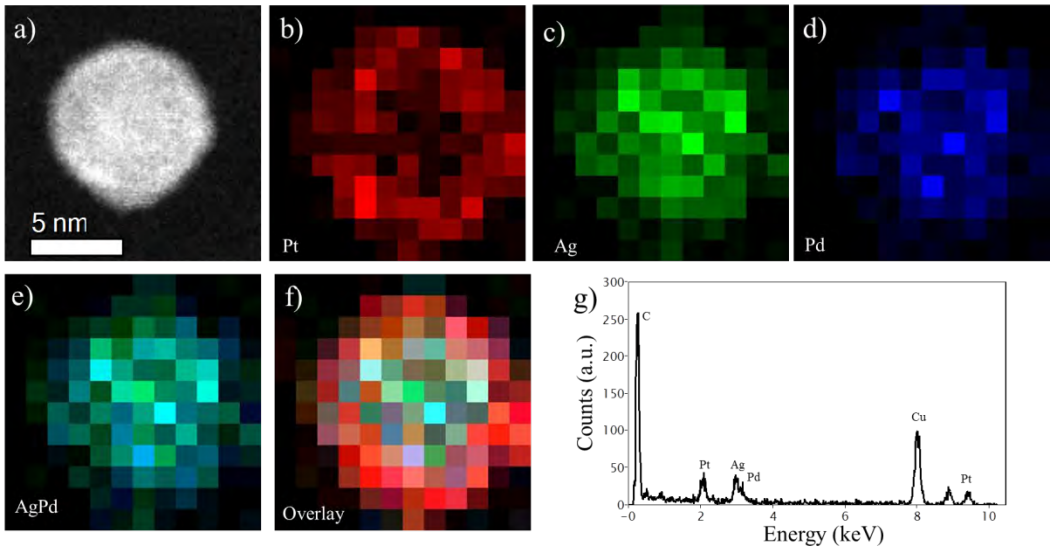

Fig. S2 EDS elemental mapping of AgPd/Pt core-shell icosahedral nanoparticles.

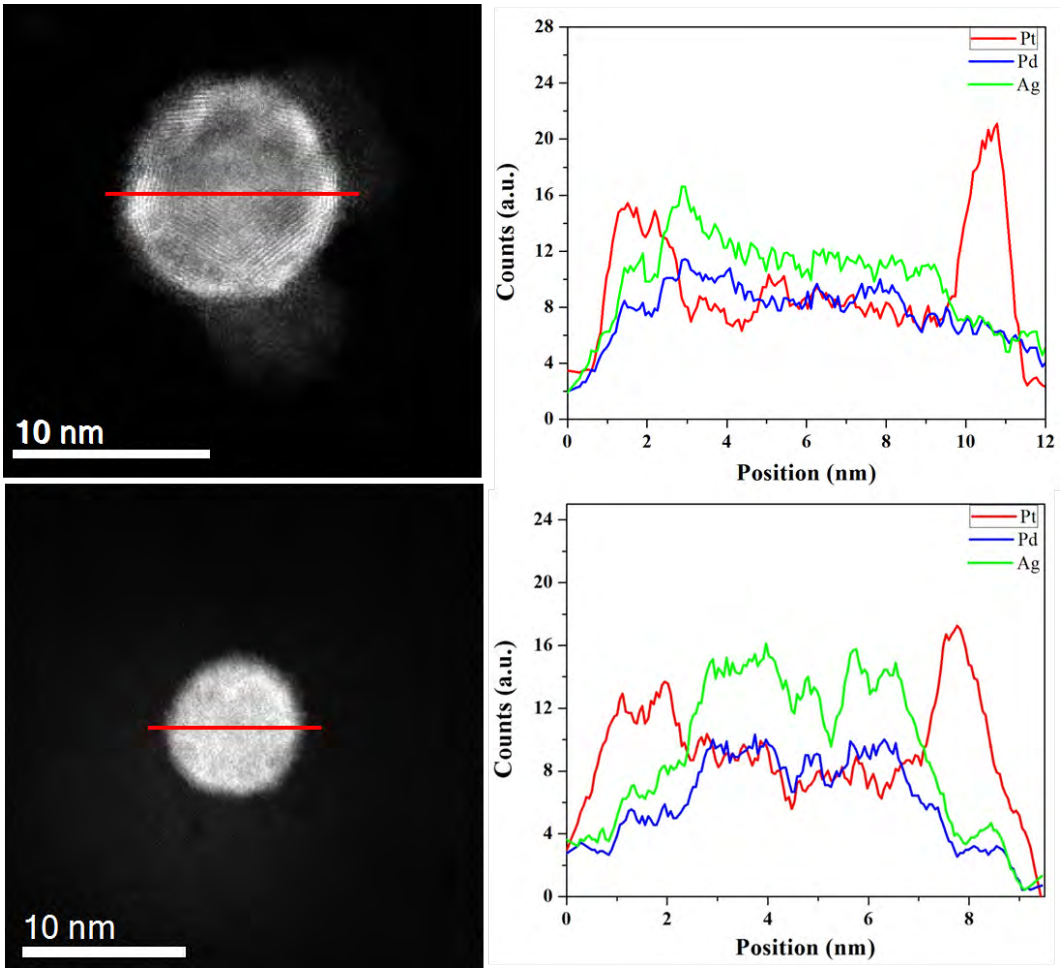

Fig. S3 EDX line scanning of the AgPd/Pt icosahedral core-shell nanoparticles.

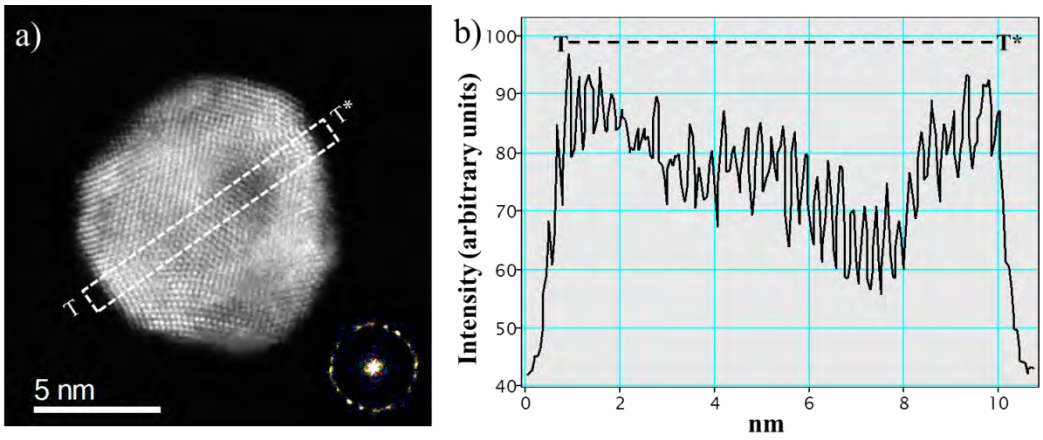

Fig. S4 Cs corrected HAADF-STEM image of (a) AgPd/Pt nanoparticles with a Pt rich shell and AgPd rich core, (b) intensity profile (in arbitrary units) of the area marked in a) showing the difference in the intensity due to the facts that $Z_{Pd} < Z_{Ag} < Z_{Pt}$.

Density Functional Calculations for RNH_2 Adsorption on Pd and Ag surfaces:

The DFT calculations were performed with DACAPO, a density functional theory (DFT) code. The electron-ion interactions were accounted through ultrasoft pseudopotentials, while the valence electrons were treated within the generalized gradient approximation (GGA) in the version of Perdew and Wang (PW91). An energy cutoff of 400 eV and a Monkhorst-Pack grid of 12x12x1 was used to satisfy the energy accuracy with an error of 10 meV. The top surface layer and the adsorbates were relaxed until the total forces were less than 0.02 eV/Angstrom. None of the structures shown magnetic behavior so that spin was ruled out. The lattice constants where taken from the calculated equilibrium distances of a periodic fcc bulk: 4.14 Angstroms for Ag, and 3.99 for Pd.

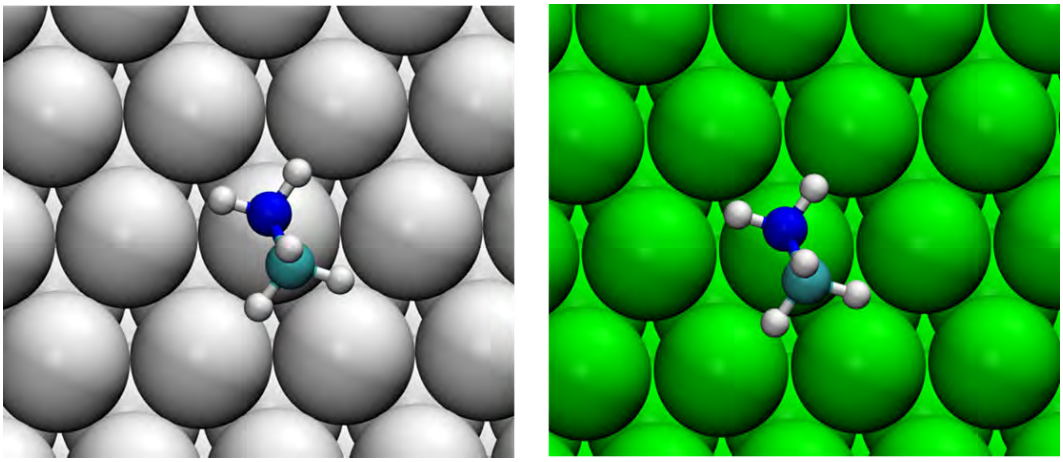

Fig. S5 Methylamine adsorption on Ag(111) (left) and on Pd(111) right at a coverage degree of 1/9.

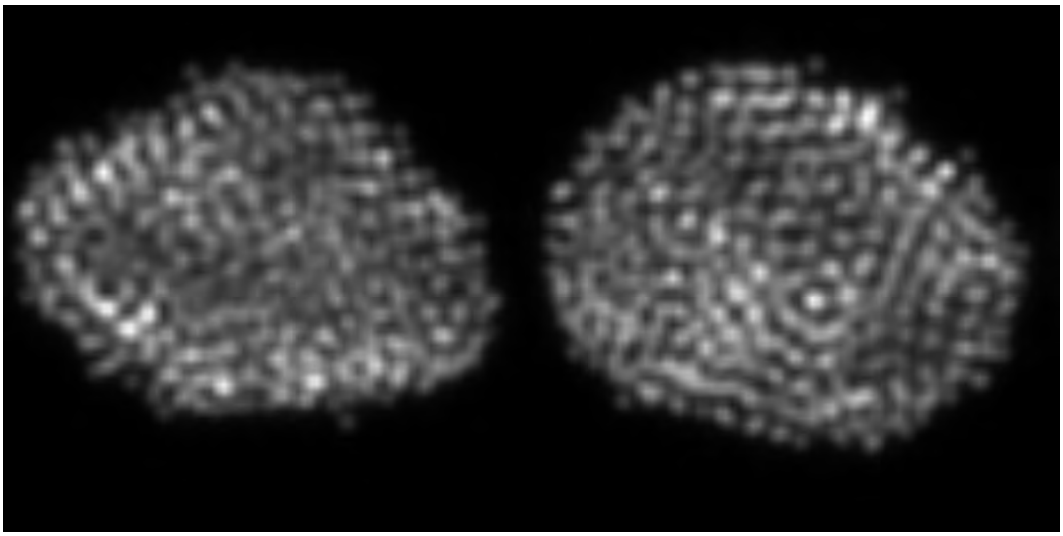

Fig. S6 STEM simulations of the same configuration shown in Fig. 6g at different orientations.