Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Revealing chemical ordering in Pt-Co nanoparticles using electronic structure calculations and X-ray photoelectron spectroscopy

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Supplementary Information

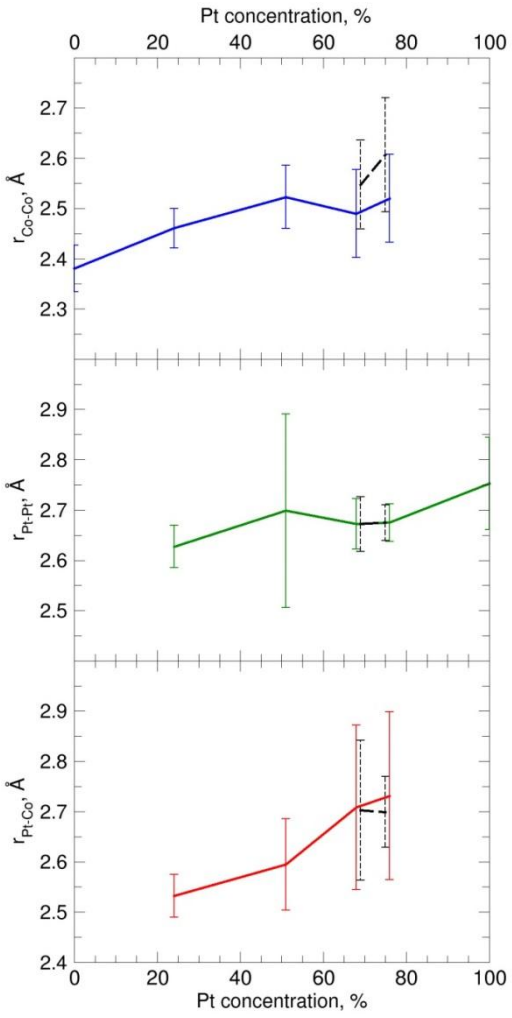


Figure S1. Calculated average nearest-neighbor distances (r_{Co-Co}, r_{Pt-Pt} and r_{Pt-Co}) in the global minimum structures of the bimetallic nanoparticles as a function of their Pt-Co composition. Colored and black dashed lines represent Pt_XCo_{79-X} and Pt_XCo_{140-X} nanoparticles, respectively. Error bars indicate the corresponding standard deviations (σ).

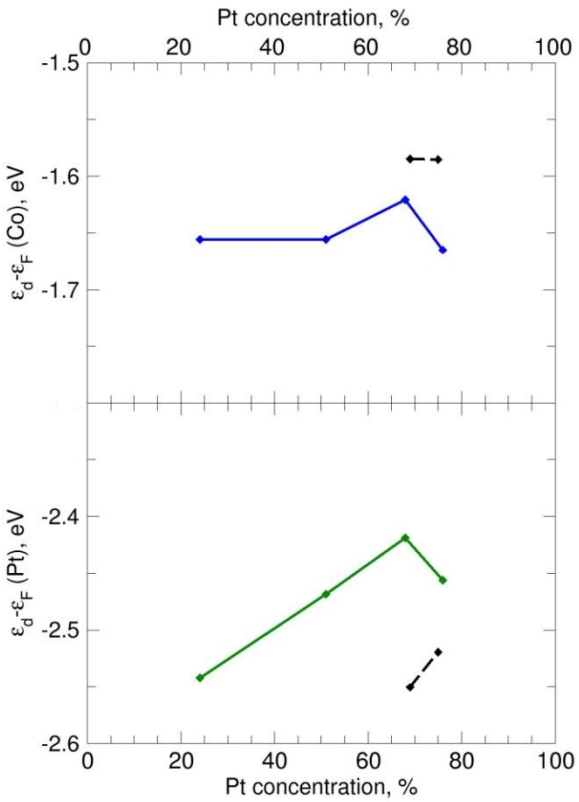


Figure S2. Calculated *d*-band center energies ε_d of all Pt and Co atoms in Pt-Co nanoparticles of various size and composition with respect to the corresponding Fermi-level values ε_F. Colored and black dashed lines show data for Pt_XCo_{79-X} and Pt_XCo_{140-X} nanoparticles, respectively.

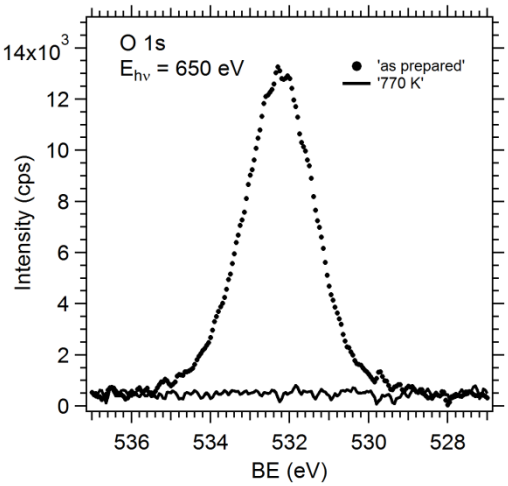
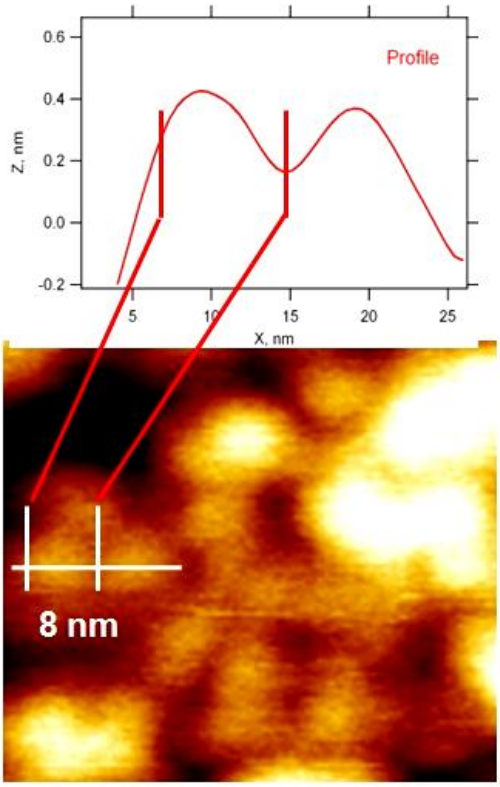
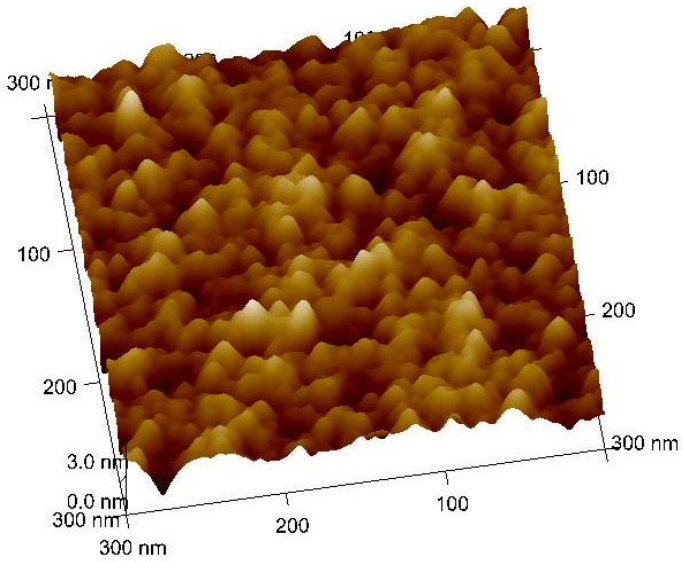


Figure S3. SXPES O 1s spectra of Pt-Co NP film, dotted line shows the spectrum of the "as prepared" sample, whereas the full line corresponds to the spectrum of the sample "after annealing".



a)



b)

Figure S4. a) AFM image of the annealed Pt-Co NP film with marked 8 nm particles and height profile; b) AFM image of the annealed PtCo NP film showing 3D structure of the catalyst film.