Electronic Supplementary Information:

Effect of Lattice Mismatch and Shell Thickness on Strain in Core@Shell Nanocrystals

Jocelyn T.L. Gamler,a Alberto Leonardi,b Xiahan Sang,c Kallum M. Koczkur,a Raymond R. Unocic,c Michael Engel,b and Sara E. Skrabalak,a,*

a. Department of Chemistry, Indiana University, 800 East Kirkwood Avenue, Bloomington, Indiana 47405, United States. E-mail: sskrabal@indiana.edu
b. Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstraße 49b, 91052 Erlangen, Germany
c. Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, One Bethel Valley Road, Oak Ridge, TN 37831, USA

**Figure S1.** TEM images of (A) Pd cubes and (B) Rh cubes used as cores.
**Figure S2.** (A) GPA colors maps which correspond to the in-plane strain ($\varepsilon_{xx}$) field from Figure 3G. (B) is the line profile of the relative deformation determined by GPA with the line profile locations indicated by the arrow in A where the start of the line profile begins at the black dot and ends at the point of the arrow.

**Figure S3.** Transversal lattice parameter deformation in Rh@Pt nanocrystals. Variation of the transversal deformation of the lattice parameter along a central line section normal to the surface as a function of the distance from the center for a set of nanocrystals with increasing surface-shell thickness ca. from 0.5 to 9 nm. The profiles have been shifted by the deformation at the center of the nanocrystal, which is shown in the inset.