Improving Quantitative EDS Chemical Analysis of alloy Nanoparticles by PCA Denoising: Part I, reducing reconstruction bias.

Murilo Moreira[1], Matthias Hillenkamp[1,2], Giorgio Divitini[3], Luiz H. G. Tizei[4], Caterina Ducati[3], Monica A. Cotta[1],Varlei Rodrigues[1,*], Daniel Ugarte[1,*]

1. *Instituto de Fisica "Gleb Wataghin", Universidade Estadual de Campinas-UNICAMP, 13083-859, Campinas - SP, Brazil*
2. *Institute of Light and Matter, Université Claude Bernard Lyon 1, CNRS, UMR5306, F-69622 Villeurbanne, France*
3. *Department of Materials Science and Metallurgy, University of Cambridge, Cambridge CB3 0FS, United Kingdom*
4. *Laboratoire de Physique des Solides, Université Paris-Saclay, CNRS, 91405 Orsay, France*

***Correspondence and requests for materials should be addressed to:**
D.U. (email: dmugarte@ifi.unicamp.br) or to V.R. (email: varlei@ifi.unicamp.br)

Figure S1.

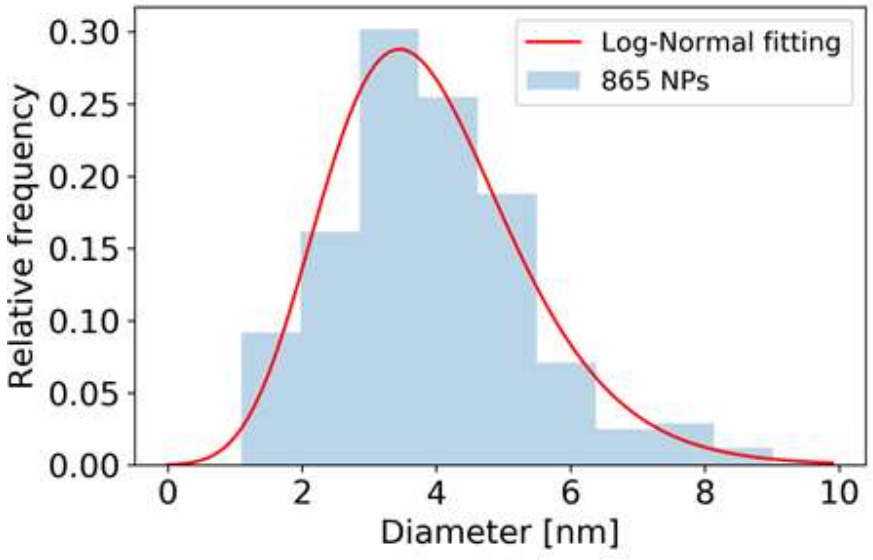

Figure S1. Typical size distribution of the alloy NP used in Experiment I, II and III as measured by TEM. The continuous curve represents a log-normal description of the distribution.

Figure S2.

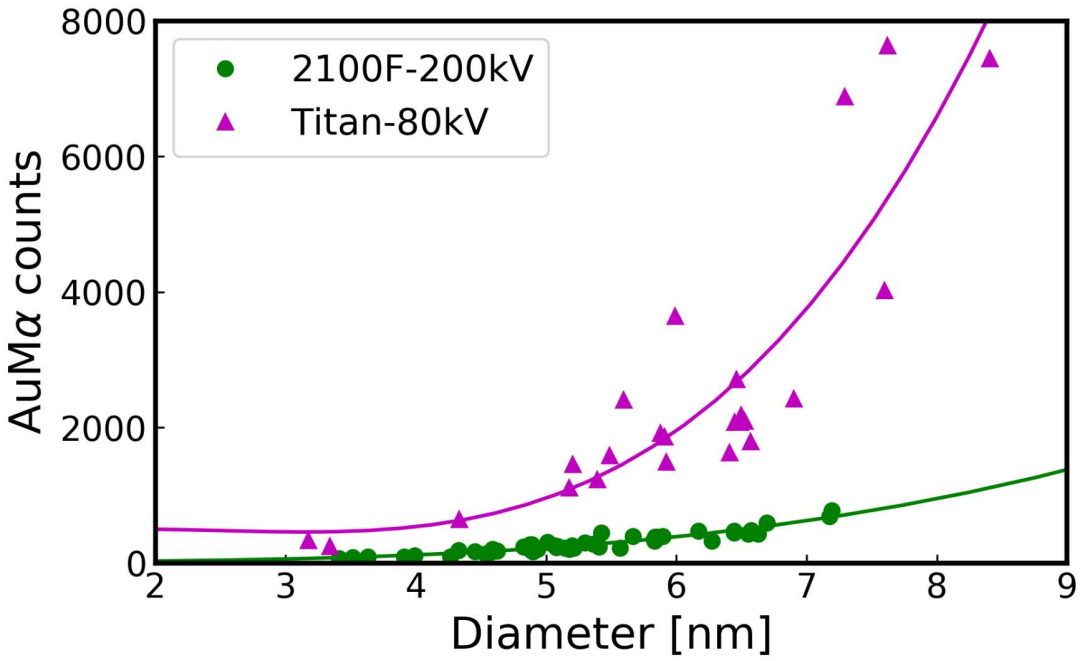

Figure S2. Integrated total counts per NP at the Au L_α peak (200 ms dwell time), as a function of NP diameter for different instruments. This allows a quick estimation of expected counts and Poisson noise for nanoparticle. A the mathematical expression describing the general tendency of the plots has been obtained by fitting the data. The observed counts as a function of NP diameter (D) can be estimated the equation below, derived from Figure S2.

for Titan-80kV, $I(D) = 38.3\ D^3 - 287.4\ D^2 + 670.7\ D$

for JEM2100F-200kV, $I(D) = 2.4\ D^3 - 6.9\ D^2 + 18.6\ D$

Figure S3.

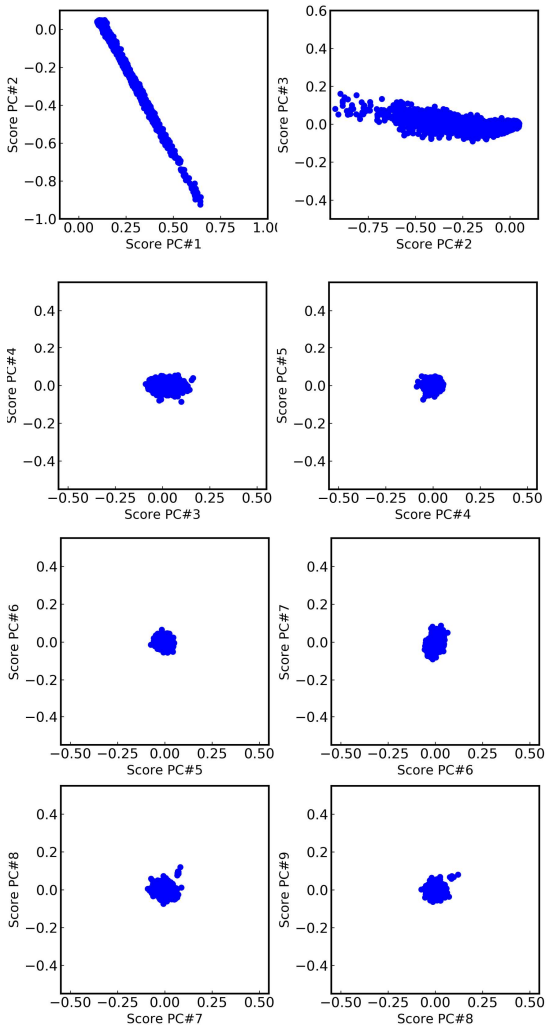

Figure S3. Cluster plot of scores for successive principal components obtained PCA processing a high SNR simulated EDS HSI of bimetallic NPs (Potapov, P., Lubk, A. (2019). Optimal principal component analysis of STEM XEDS spectrum images. *Adv. Struct. Chem. Imag.* ***5***, 4). Note that information-carrying component shows a structured anisotropic cloud (top), while noise components generate isotropic round clouds.