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Systematic Distortions in Nanoparticles as Modeled by EXAFS Analysis AARON YEVICK, ANATOLY FRENKEL, Yeshiva University — We modeled EXAFS from cuboctahedral nanoclusters with radii of 11-15 Å. Such clusters may undergo significant surface distortion under the influence of ligands, substrate and/or surface tension. These effects can reduce the average nearest neighbor distance in the cluster by 2-4% and cause enhanced disorder in the interatomic distance as a result of the stronger relaxation of surface bonds relative to the cluster interior. Such effects can degrade the accuracy of EXAFS analysis where the standard approach is to assume a quasi-Gaussian distribution of nearest neighbors. We present a quantitative analysis of the systematic errors that arise in EXAFS measurements as a result of neglecting such surface-induced disorder, in particular the measurement of the coordination number, which could be affected by up to 6%.

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