Supplementary Material

Visualizing Screening in Noble-Metal Clusters: Static vs. Dynamic

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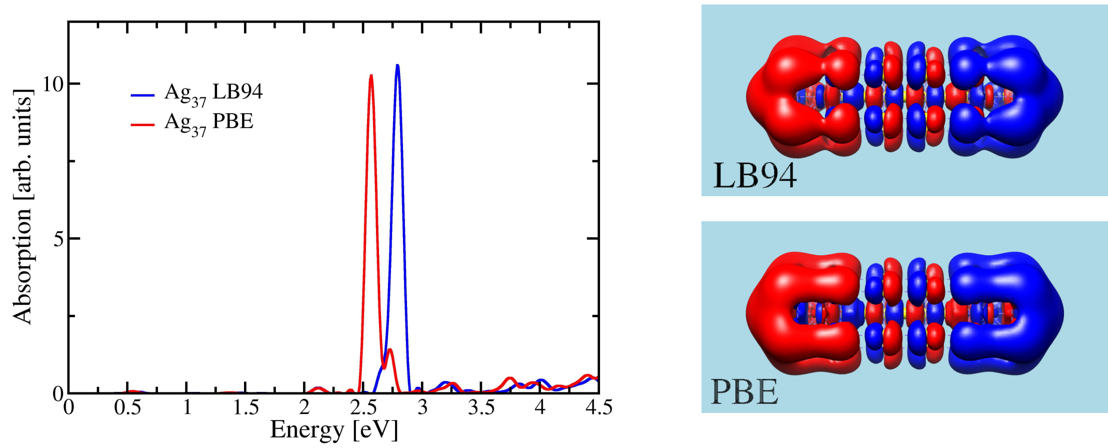
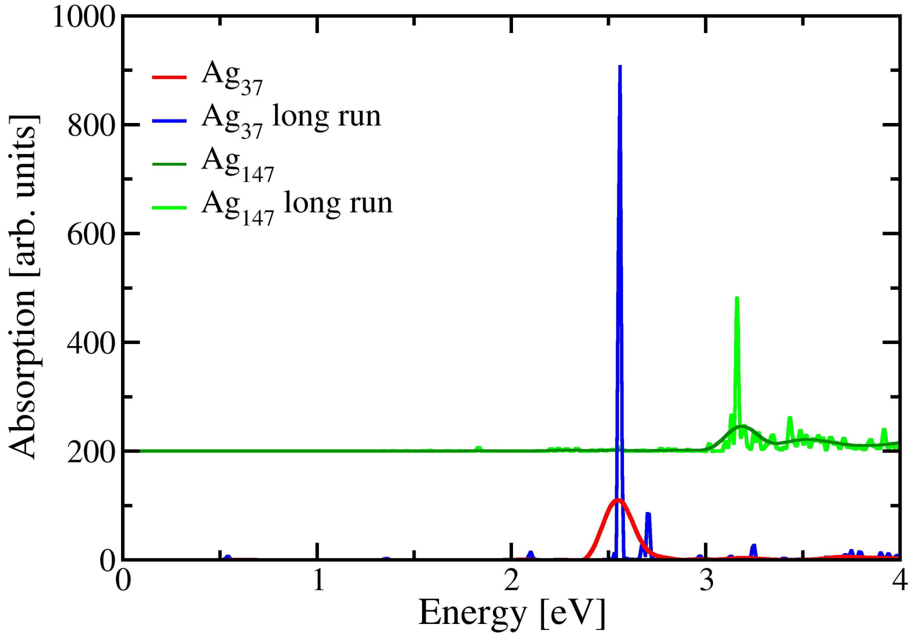
Comparison of functionals



Supplementary Figure S1. LHS: Optical absorption spectra of a 37-atom silver rod comparing PBE as used in the article with the long-range-corrected LB94. Apart from the well-known blue-shift of the SPR with LB94,[1] the qualitative result remains unchanged. RHS: reconstructed modes of density oscillation at the respective energies for the LB94 and the PBE calculation (maximum of the density oscillations), the iso value is 3×10^{-6}.

Longer time evolutions for better resolution of modes



Supplementary Figure S2. Optical absorption spectra of a 37-atom silver rod and of the icosahedral 147-atom silver cluster. The two systems are the smaller versions of the two structures used in the present paper, the quasi-spherical icosahedral Ag_{309} and the nanorod Ag_{263}. The "normal" evolution time was 25 fs, the "long run" was 250 fs. Note that below the main peak features, only few, and very weak, absorption features are visible in all the cases.

References

(1) Aikens, C. M.; Li, S.; Schatz, G. C. From Discrete Electronic States to Plasmons: TDDFT Optical Absorption Properties of Ag n (n = 10, 20, 35, 56, 84, 120) Tetrahedral Clusters. *J. Phys. Chem. C* **2008**, *112*, 11272.