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Surface plasmons in quantum-sized noble-metal clusters: TDDFT quantum calculations and the classical picture of charge oscillations

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Icosahedra Ag₁₄₇ and Au₁₄₇

Ag₁₄₇

Au₁₄₇

Animation A: Isosurfaces of the difference between time-dependent density and ground state density $\rho(\mathbf{r}, t) - \rho_{\text{gs}}(\mathbf{r})$, at a value of $1 \times 10^{-5} \text{ \AA}^{-3}$, corresponding to Fig. 2 of the article: Icosahedral Ag₁₄₇ (left) and Au₁₄₇ (right). For Ag₁₄₇, one period of the approximately periodic movement is shown, whereas for Au₁₄₇, a relatively arbitrary interval was chosen out of the entirely non-periodic dynamics. The shown interval starts after about 25 fs of time evolution (see Fig. 2 of the article).

Nanorods Ag₃₇ and Au₃₇

Ag₃₇

Au₃₇

Animation B: Time-dependent density $\rho(\mathbf{r}, t) - \rho_{\text{gs}}(\mathbf{r})$, at a value of $1 \times 10^{-4} \text{ \AA}^{-3}$, corresponding to Fig. 3 of the article: pentagonal nanorods Ag₃₇ (left) and Au₃₇ (right). For Ag₃₇, one period of the approximately periodic movement is shown, whereas for Au₃₇, a relatively arbitrary interval was chosen out of the entirely non-periodic dynamics. The shown interval starts after about 25 fs of time evolution. Red = positive, blue = negative difference $\rho(\mathbf{r}, t) - \rho_{\text{gs}}(\mathbf{r})$.

Monatomic chain Ag₇

Animation C: Time-dependent density corresponding to Fig. 5 of the article: monatomic chains Ag₇ for an excitation along the axis (left) and perpendicular to the axis of the chain (right). Shown is the difference between time-dependent density and ground-state density $\rho(\mathbf{r}, t) - \rho_{\text{gs}}(\mathbf{r})$ (red = positive, blue = negative), at a value of $1 \times 10^{-5} \text{ \AA}^{-3}$.

Screening by d electrons: rod Ag₃₇

Animation D: Time-dependent density corresponding to Fig. 6 of the article: pentagonal nanorod Ag₃₇ for an excitation along the axis for different isovalues as indicated, in units of Å⁻³.

Comparison Ag vs. Na (no d electrons)

Animation E: Time-dependent density corresponding to Fig. 7 of the article: pentagonal nanorod Ag₃₇ for an excitation along the axis for different isovalues as indicated, in units of \AA^{-3} , compared with a 216-atom sodium rod.