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Surface Plasmons in Quantum-Sized Noble-Metal Clusters: Quantum Calculations and the Classical Picture of Charge Oscillations HANS-CHRISTIAN WEISSKER, CNRS - CINAM, Centre Interdisciplinaire de Nanoscience de Marseille, XOCHITL LOPEZ-LOZANO, Department of Physics and Astronomy — The University of Texas at San Antonio One UTSA Circle, San Antonio, TX 78249 — The localized surface-plasmon resonance (LSPR) in metal clusters corresponds to a collective charge oscillation of quasi-free electrons of the metal. We use the real-time formulation [1] of time-dependent density-functional theory (TDDFT) with pseudopotentials to study the correspondence and differences of the quantum calculations with the classical picture. By means of animations, we discuss the real-time evolution of the electronic density for different geometries. While there is a clear correspondence between the overall picture of a charge oscillation and the actual dynamics in quantum-sized clusters, the situation is much more intricate owing to quantum effects and the atomistic inhomogeneity of the cluster. A fine pattern is present over the volume of the cluster even at moments of zero overall polarization. The difference between Ag and Au is clearly visible. Finally, we discuss the question of collective vs. molecular-like transitions; even for single transitions, the dynamics of the total density can be similar to the picture of a charge oscillation.

[1] Yabana, K.; Bertsch, G. F., Phys. Rev. B 54, 4484 (1996).

[2] Weissker, H.-Ch., Whetten, R.L., and López-Lozano, X.; PCCP 16, 12495 (2014).

[3] López-Lozano, X.; Barron, H.; Mottet, C.; Weissker,

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