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Optical Properties of Free and Embedded Small Nanoparticles

JUAN IDROBO, Vanderbilt University and Oak Ridge National Laboratory

It is well known that the absorption spectra, as well as the effective dielectric function, of nanoparticles in vacuum or surrounded by a dielectric medium can be obtained by classical Mie and Maxwell-Garnett theories. A limit as to how the particles can be for the theory to apply has not been established. Here I present theoretical results on the optical properties of small Ag, Au, and Si and Ge nanoparticles with tens of atoms in vacuum and in an embedded dielectric medium obtained from first-principles density-functional calculations. In particular, I will discuss the role that *d*-electron play on the optical properties of Ag and Au nanoparticles, and the cases when classical Mie and Maxwell-Garnett theories can be applied for nanoparticles of just few atoms in size and whose atoms are in bulk-like and not bulk-like positions. Comparison will be made for nanoparticles in vacuum and embedded in an alumina matrix. The quantum-mechanical results indicate that small nanoparticles in alumina can have an imprint on the effective dielectric function that is several times larger than would be predicted by Maxwell-Garnett theory for same-size particles. This work was supported by a GOALI NSF grant, DOE, the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, and Alcoa Inc. Collaborators: S. Ögüt, K. Jackson, J. Jellinek, A. Halabica. R. F. Haglund, R. Magruder, S.J. Pennycook and S.T. Pantelides.