Abstract Submitted
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First Principles Absorption Spectra of Si_n ($n = 20 - 28$) Clusters: TDLDA versus Predictions from Mie Theory[1] KOBLAR JACKSON, Central Michigan University, JUAN C. IDROBO, SERDAR OGUT, University of Illinois at Chicago, MINGLI YANG, Central Michigan University — First-principles absorption spectra calculated within the time- dependent local-density approximation for Si_n ($n = 20 - 28$) clusters reveal that prolate and compact clusters have distinct shape signatures, but no clear size dependence for a given shape.[2] The shape dependence and size independence of the spectra and most of the peak positions and intensities can be explained remarkably well within the *classical* Mie theory, developed for light absorption by *metallic* particles using the *bulk* dielectric function of Si. Moreover, the experimental spectrum of Si_{21} is in very good agreement with the theoretical spectrum of the prolate cluster, which is lower in energy than the compact one at this size.

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[2]Idrobo, Jackson, Yang, and Ogut, Phys. Rev. B **74**, 153410 (2006)

Serdar Ogut
University of Illinois at Chicago

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