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)