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First Principles Computation of Optical Response in Silicon Nanostructures SEBASTIEN HAMEL, ANDREW WILLIAMSON, LLNL, HUGH WILSON, FRANCOIS GIGY, GIULIA GALLI, UC Davis, ED RATNER, DAN WACK, KLA Tencor, LLNL TEAM, UC DAVIS TEAM, KLA TENCOR TEAM — In the next few years, the typical size of finFET devices used in the microchip industry is expected to be of the order of a few nanometers. This poses formidable challenges, including for optical metrology, i.e. for the development of appropriate tools and techniques based on optical response, to monitor and validate the growth of silicon nanostructures. Current optical metrology tools are based on the assumption that in Si finFETs the dielectric response is piece-wise constant and equal to the bulk value. Such an assumption is expected to break down for sizes smaller then 10 nm, where the dielectric response of Si nanostructures may substantially deviate from that of the bulk. We present an analysis of the dielectric properties of Si slabs, spheres and rods as a function of size and shape, based on first principles, Density Functional Theory calculations. In particular, we discuss the relative influence of quantum confinement and surface effects, and propose a way to monitor dielectric properties changes at the nanoscale, based on the definition of local dielectric response functions.

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