Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Efficient calculations of the dielectric response in semiconductor nanostructures for optical metrology HUGH WILSON, GIULIA GALLI, FRANCOIS GYGI, University of California, Davis, SEBASTIEN HAMEL, ANDREW WILLIAMSON, Lawrence Livermore National Laboratory, ED RATNER, DAN WACK, KLA-Tencor — The ability to predict the optical and dielectric properties of semiconductor nanostructures is highly desirable, in order to efficiently couple theory and experiment in the characterization and design of nanostructured materials. For example, in designing optimal procedures for optical metrology, the knowledge of the full dielectric matrix of nanostructures as a function of size and shape would be desirable. However, methods based on Density Functional Theory (DFT) are only computationally feasible for sizes below 2 nm and it is still difficult to extend them to the 5 - 25nm size regime of interest to many experiments. In order to make contact between theory and experiment for this important class of systems, we have developed computational techniques based on the empirical pseudopotential method (EPM). Here we compare EPM and DFT results for small nanostructures and we then use EPM results to discuss the properties of Si spheres and rods in the larger size regime.

Hugh Wilson
University of California, Davis

Date submitted: 20 Nov 2006 Electronic form version 1.4