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Optical properties of real surfaces: local field effects at oxidized Si(100)(2x2) computed with an efficient numerical scheme[1] LUCIA CARAMELLA, GIOVANNI ONIDA, Physics Dept. University of Milano (Italy), FABIO FINOCCHI, Institut des Nanosciences de Paris (INSP) (France), LUCIA REINING, FRANCESCO SOTTILE, Laboratoire des Solides Irradiées CNRS-CEA, Ecole Polytechnique (France) — We show the application of an efficient numerical scheme to obtain the independent-particle dynamic polarizability matrix $\chi^{(0)}(\mathbf{r}, \mathbf{r}', \omega)$, a key quantity in modern *ab initio* excited state calculations. The method has been applied to the study of the optical response of a realistic oxidized silicon surface, including the effects of the local fields. The latter are shown to substantially increase the surface optical anisotropy in the energy range below the bulk bandgap. Our implementation in a large-scale *ab initio* computational code allows us to make a quantitative study of the CPU time scaling with respect to the system size, and demonstrates the real potential of the method for the study of excited states in large systems.

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