

Abstract Submitted
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Band structure calculations of the surface linear optical response of the clean and hydrogenated Si(100) surface¹ B. MENDOZA, N. ARZATE, Centro de Investigaciones en Optica, F. NASTOS, J. SIPE, Dept. of Physics, U. of Toronto — We calculate the reflectance anisotropy (RA) and the reflectance difference (RD) spectra for a clean Si(100) surface and two H covered Si(100) surfaces. The clean surface we consider is a 2×1 surface reconstruction characterized by a tilted dimer formed between the two top-most Si atoms. One of the H covered surfaces is a monohydride surface in which the two dangling bonds of the dimer are H saturated (rendering a flat dimer), and the other is a dihydride surface in which the H saturates each of the two dangling bonds leading to a bulk ideally terminated surface. This dihydride surface is thought to be created if enough H is added to the surface. The optical response is calculated both with pseudopotential and all-electron LAPW band structures including a scissors shift, and compared. In the pseudopotential we neglect the non-local contribution to the momentum matrix elements. We contrast the two methods and trace their differences to the physics involved in each one. Finally, we compare our results with available experimental measurements on this surface.²

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²Yves Borensztein, private communication

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