Numerical model studies of confinement effects and optical properties of multilayer slabs of silicon

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The surface properties of $Si(111) : H$ can be modeled by means of slabs with increasing number of layers. Electronic orbitals obtained from previous ab initio calculations [1] show patterns of periodicity due to confinement effects. These also influence the optical properties of the surface when it is excited by visible light. The slab model and results are modeled with a finite periodic potential parametrized with information about atomic radii and electron binding energies. The model is then solved numerically to obtain electronic energy levels and the shape of layer orbitals. The procedure provides insight on trends in confinement and optical absorption intensities, and a straightforward procedure to also explain the effect of adsorbed species. Calculated results include HOMO-LUMO excitation energies, and intensities of absorption from calculated electric transition dipoles and density of states.

1. D. S. Kilin and D. A. Micha, Chem. Phys. Lett. **461**, 266 (2008).

2. P. W. Atkins and R. S. Friedman "Molecular Quantum Mechanics", 3rd edition (Oxford Univ. Press, 1997), Chap. 12

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