

PHD thesis:

“Study of the optical properties of interfaces, surfaces of nanostructures”

(cotutelle between the University of Modena and Reggio Emilia and the Ecole Polytechnique)



UNIVERSITÀ DEGLI STUDI
DI MODENA E REGGIO EMILIA



POLYTECHNIQUE



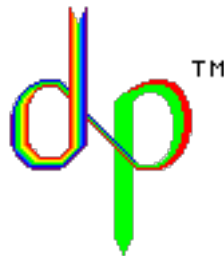
Ab-initio approach (DFT and TDDFT)

Ab-initio calculation are useful to investigate and understand the role played by particular effects in the nanostructures.

You can create ad-hoc systems in order to separate their contributions and investigate them separately

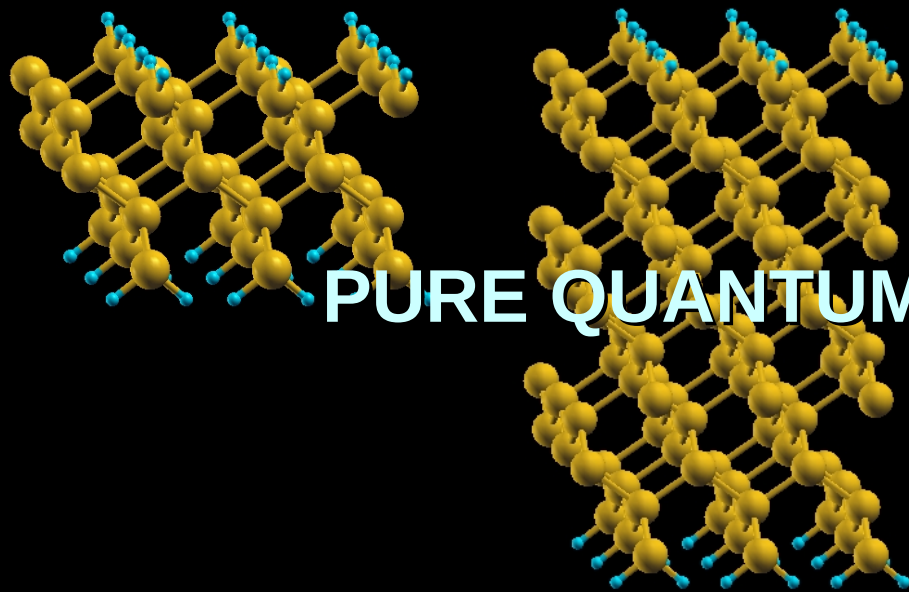


abinit.org

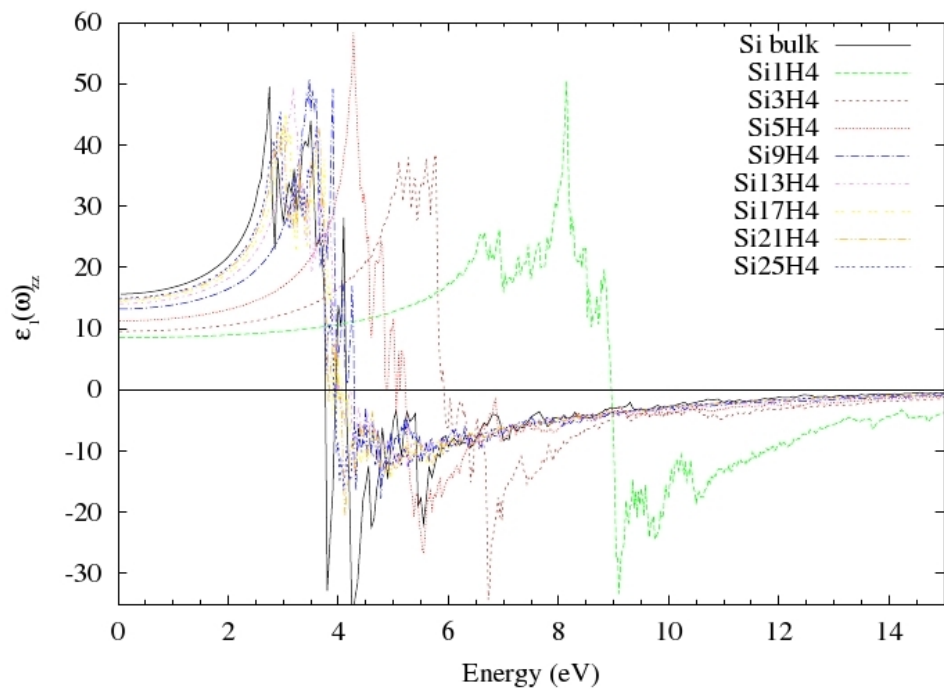
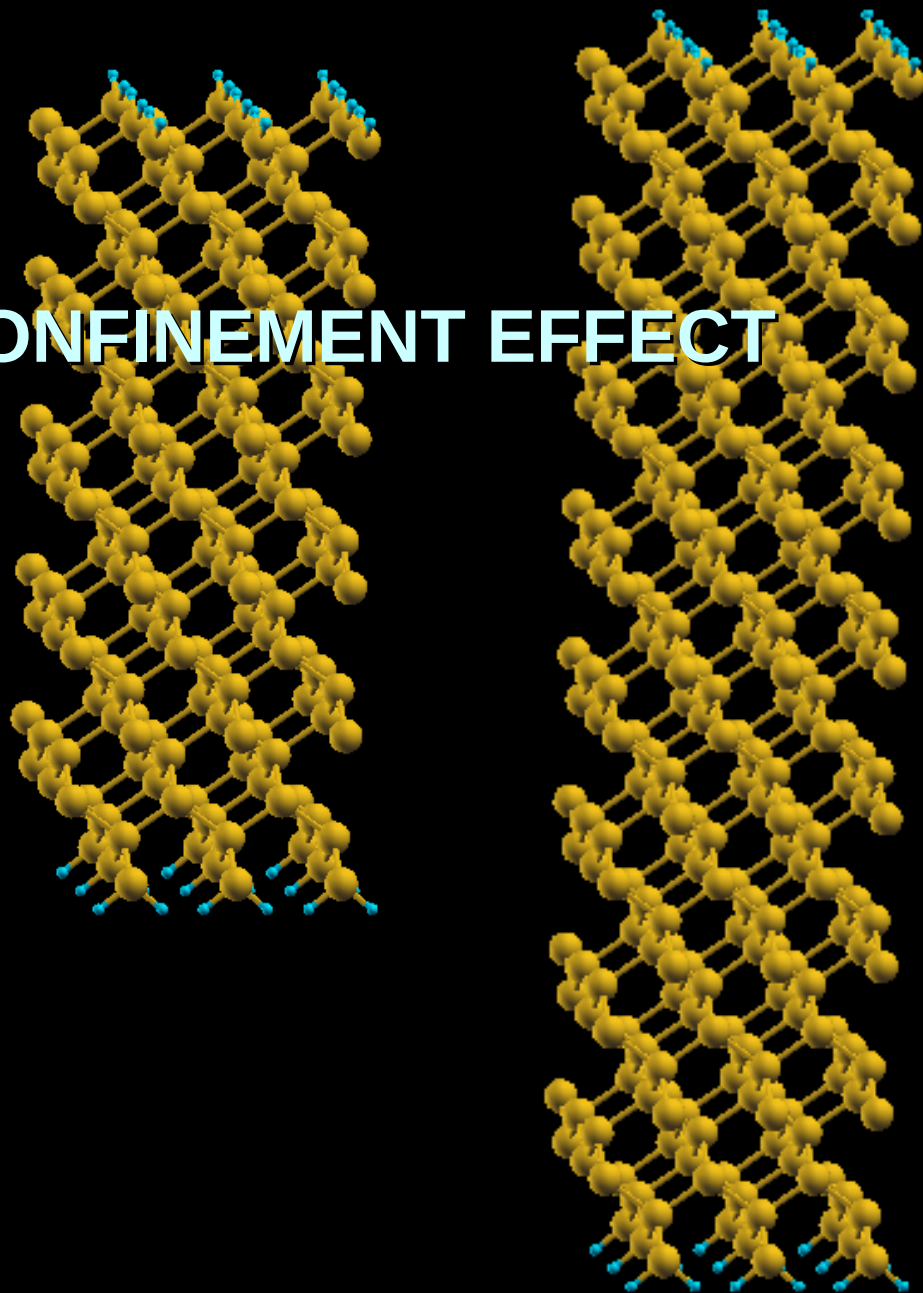


2light code

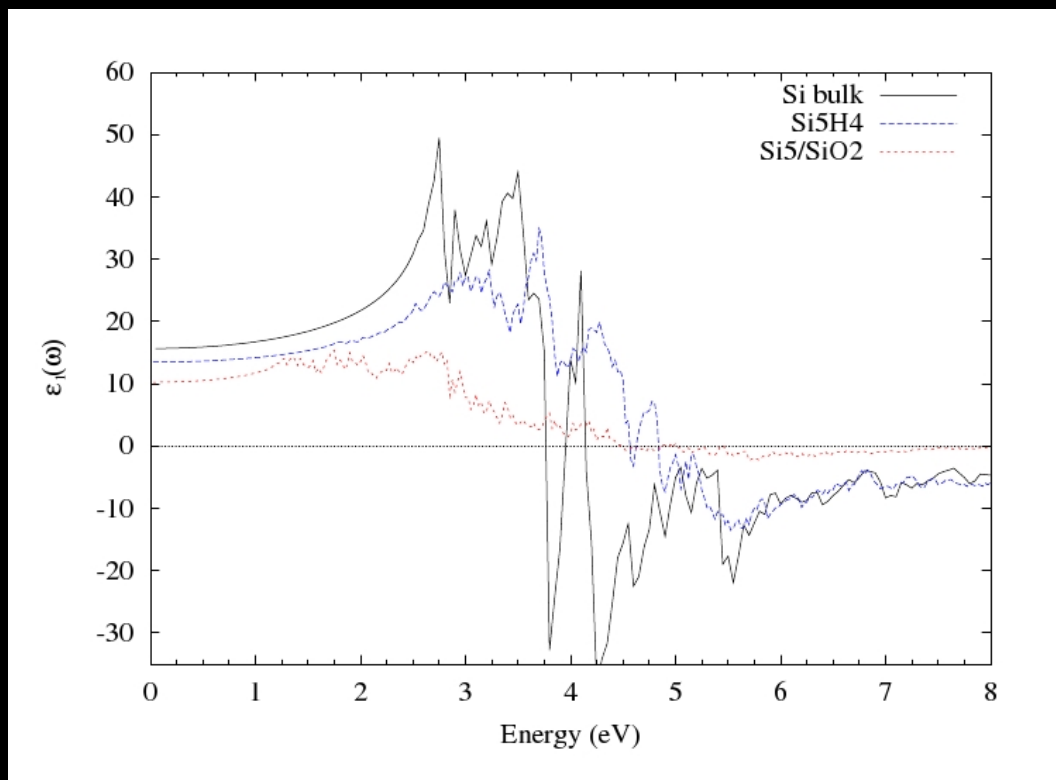
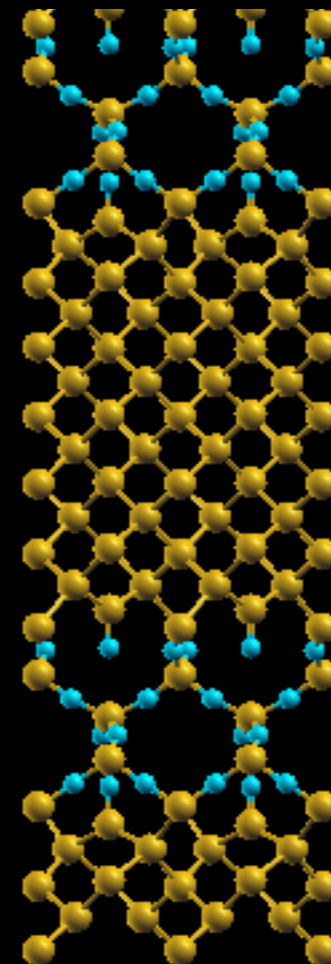
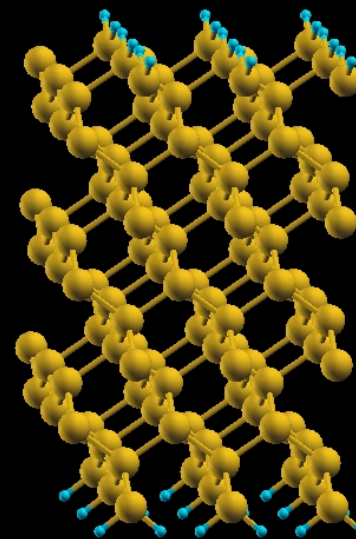
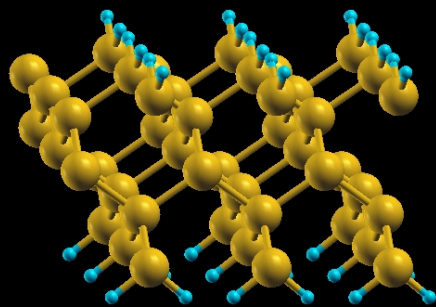
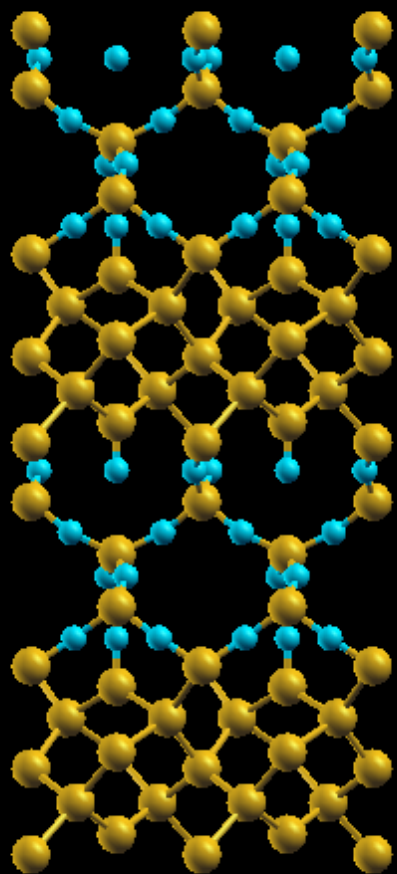
Example: study of the Si/SiO₂ multilayers



PURE QUANTUM CONFINEMENT EFFECT



INTRODUCTION OF THE INTERFACE EFFECTS



Example: study of the Si/CaF₂ multilayers

T. F. Heinz, F. J. Himpsel, and
E. Palange,
Phys. Rev. Lett. 63, 644 (1989)

Determination of the interface configuration

