O 2 Invited talk Pulci

Time: Monday 10:15–11:00 Room: TRE Phys

Invited Talk O 2.1 Mon 10:15 TRE Phys

Ab initio description of electronic excitations at surfaces — •Olivia Pulci — ETSF, CNR-INFM, Dept. of Physics University of Rome Tor Vergata, Rome, ITALY

Structural, electronic and optical properties of complex systems are nowadays accessible thanks to the impressive development of theoretical approaches and computer power.

Nanostructures, surfaces and even biological systems can now be studied within ab-initio methods fully including exchange and correlation effects.

We will review the Many-Body Perturbation Theory based on the Green's function formalism, and present examples of GW and excitonic calculations for systems ranging from nanocrystals to liquid water.

Applications to the study of the band structure, electron affinity and optical properties of diamond, silicon, and germanium surfaces will be discussed in details.