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Curriculum Vitae

I got my Ph. D. in Physics in 2006, at University of Rome "Tor Vergata". I have been post-doc at NNL-CNR in Lecce (2006-2008), at the Universidad del Pais Vasco (2008-2010), and at present I am a researcher at the Italian Institute of Technology - IIT in Rome.

Research Interest

My research activity, in the field of theoretical solid state physics, focuses on ab initio study of reduced-dimensionality systems (surfaces, interfaces, nanocrystals) and of organic-inorganic hybrid systems, paying particular attention to their applications in nanotechnology. Methods are mainly based on Density Functional Theory, both with all-electron, localized basis

and pseudopotential-plane waves approaches. Excited properties methods rely on TDDFT, and Many Body Perturbation Theory based techniques including GW, sc-COSHEX, BSE.

Current Research Projects

My work is at present focused on two main research lines. The first one is the investigation, via classical molecular dynamics, of membrane proteins, to understand their behaviour in presence of ligands, and of protein-protein interaction. The second topic is related to material science, in particular nanoscience, with the study via MD and ab initio electronic methods of metal nanostructures and their interaction with organic and biological molecules.

Recent Publications

1. L. Chiodo, T. E Malliavin, L. Maragliano, G. Cottone, G. Ciccotti "Molecular dynamics simulations of a new model of human $\alpha 7$ nicotinic receptor", in preparation.
2. F. Gentile, M. Monteferrante, L. Chiodo, A. Toma, M. L. Coluccio, G. Ciccotti, E. Di Fabrizio, "Electroless formation of super-cluster of metal-atoms: an experimental and molecular dynamics approach", Mol Phys 112 (9-10), 1375-1388 (2014).
3. L. Chiodo, G. Giorgi M. Palumbo, K. Yamashita, A. Rubio, "Excitons at the molecular-(001) anatase interface and ab initio charge transfer", to be submitted.

4. C. Violante, L. Chiodo, A. Mosca Conte, F. Bechstedt, O. Pulci, "Si(111)2x1 surface isomers: DFT investigations on stability and doping effects", Surf. Sci 621, 123-127 (2014) , <http://dx.doi.org/10.1016/j.susc.2013.11.006>
5. P. Gargiani, S. Lisi, M. G. Betti, A. Taleb, F. Bertran, P. Le Fevre, L. Chiodo, "Orbital dependent Rashba splitting and electron phonon coupling of 2D Bi phase floating on Cu(100) surface", J. Chem. Phys. 139, 184707 (2013), <http://dx.doi.org/10.1063/1.4828865>
6. G. Roma, L. Chiodo, "Selenium adsorption on Mo(110): a first principles investigation", Phys. Rev. B 87, 245420 (2013).
7. A. Tanwar, E. Fabiano, P. E. Trevisanutto, L. Chiodo, F. Della Sala, "Accurate ionization potential of gold anionic clusters from density functional theory and many-body perturbation theory", Eur. Phys. J. B 86, 161 (2013).
8. L. Chiodo, A. Iacomino, M. Palummo, A. Rubio, "Titania nanostructures electronic and optical response by high-level ab-initio computational approaches", in "Handbook of Functional Nanomaterials", Nova Science Publishers, Ltd. (New York – USA) (2014).
9. M. Palummo, G. Giorgi, L. Chiodo, A. Rubio, and K. Yamashita "Two dimensional-like TiO₂ nanostructures: electronic and optical properties from first-principles". J. Phys. Chem. C 116, 18495-18503(2012) DOI: 10.1021/jp304618n
10. G. Mallocci, L. Chiodo, A. Rubio, A. Mattoni, "Structural and Optoelectronic Properties of Unsaturated ZnO and ZnS Nanoclusters", J. Phys. Chem. C, 116, 8741-8746 (2012).
11. L. Chiodo, A. Massaro, S. Laricchia, F. Della Sala, R. Cingolani, M. Salazar, A. H. Romero, A. Rubio, "Characterization of TiO₂ Atomic Crystals for Nanocomposite Materials Oriented to Optoelectronics", Optical and Quantum Electronics (2012) (doi: 10.1007/s11082-012-9559-y).
12. L. Chiodo, L. A. Constantin, E. Fabiano, and F. Della Sala, "Nonuniform scaling applied to surface energies of transition metals", to be printed, Phys. Rev. Lett. 108, 126402 (2012).
13. L. Chiodo, M. Salazar, A. H. Romero, S. Laricchia, F. Della Sala, and A. Rubio, "Structure, electronic and optical properties of TiO₂ tyatomic clusters: an ab initio study", J. Chem. Phys. 135, 244704 (2011) (doi: 10.1063/1.3668085).
14. G. Giorgi M. Palummo, L. Chiodo, and K. Yamashita, "Excitons at the (001) surface of anatase: Spatial behavior and optical signatures", Phys. Rev. B 84, 073404 (2011) (BR).
15. L. A. Constantin, L. Chiodo, E. Fabiano, I. Bodrenko, and F. Della Sala,

“Correlation energy functional from jellium surface analysis”, Phys. Rev. B 84, 045126 (2011).

16. L. Chiodo, J. M. García-Lastra, A. Iacomino, S. Ossicini, J. Zhao, H. Petek, A. Rubio, “Self-energy and excitonic effects in the electronic and optical properties of TiO₂ crystalline phases”, Phys. Rev. B 82, 045207 (2010).

Related Links

[my webpage at IIT](#)

[my webpage at ETSF Scientific Development Centre](#)