

## Scientific Curriculum Vitae

### Letizia Chiodo

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**Current Position: Associate Professor (Professore II Fascia)**, Università Campus Biomedico di Roma (UCBM), Facoltà Dipartimentale di Ingegneria, PHYS-04/A (Theoretical Physics of Matter, Models, Mathematical Methods and Applications), since February 2023.

#### **Previous Professional Appointments**

March 2020 - January 2023: Assistant Professor (RTDb), Università Campus Biomedico di Roma (UCBM), Facoltà Dipartimentale di Ingegneria, FIS03, 02/B2 (Theoretical Condensed Matter Physics)

January 2016 - February 2020: Assistant Professor (RTDa), Università Campus Biomedico di Roma (UCBM), Facoltà Dipartimentale di Ingegneria, FIS03, 02/B2 (Theoretical Condensed Matter Physics).

January 2012 - July 2015: Post Doc Researcher at IIT – Istituto Italiano di Tecnologia, Center for Life Nano Science @Sapienza and host at GCI-Computational Physics Group, Physics Department, University of Rome ‘La Sapienza’.

February 2010 - December 2011: Post Doc Researcher at IIT – Istituto Italiano di Tecnologia, Center for Biomolecular Nanotechnologies, Via Barsanti, 73010, Arnesano (Le), Italia.

October 2009, March 2010: Visiting Professor at Physics Department of University of Cagliari (UNICA), group of Prof. Luciano Colombo, awarded by the Visiting Professor program University of Cagliari (UNICA) 2009/2010, for 1 month visit.

November 2008 - January 2010: UPV/EHU Granted Post-Doctoral Fellowship at Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF) Departamento de Fisica de Materiales, Unidad de Materiales Centro Mixto CSIC-UPV/EHU, Universidad del Pais Vasco.

June 2008 - October 2008: Invited Professor at Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF) Departamento de Fisica de Materiales, Unidad de Materiales Centro Mixto CSIC-UPV/EHU, Universidad del Pais Vasco.

February 2006 - June 2008: Post-Doctoral Fellowship in the framework of the European Project SA-NANO, at National Nanotechnology Laboratory NNL, CNR-INFM, Lecce.

November 2005 - January 2006: Collaboration Contract at National Nanotechnology Laboratory, CNR-INFM, Lecce.

#### **Education**

November 2002 - October 2005: Ph.D. student at Physics Department, University of Rome ‘Tor Vergata’. **Ph.D. Thesis title:** ‘Ab initio study of electronic and optical properties of metallic surfaces with adsorbates’. Advisor: Prof. R. Del Sole.

May 2002: Physics Degree (110/110) magna cum laude at University of Rome ‘La Sapienza’. **Thesis title:** Electronic states of vicinal surfaces: a photoemission study of Cu(119). Advisor: Prof. M.G.Betti.

July 1997: High School Degree (60/60) at Liceo-Ginnasio Statale ‘P. Albertelli’, Rome.

#### **Grants, Prizes and Awards**

- European Commission Innovation Radar: ‘Models and simulations bridging the magneto dynamics and cardiology tools towards the investigation of cardiac turbulence’ activity selected, within the MUQUABIS project.

- European Commission Innovation Radar: ‘Multipurpose imaging system for bio imaging and remote quantum sensing via ‘undetected photons’ techniques’ activity selected, within the MUQUABIS project.

- awarded by the Visiting Professor program of University of Cagliari (UNICA) 2009/2010, for 1 month visit, with the project ‘Ab initio methods for electronic and optical properties in solid state theory, and their application to the study of dye-sensitized zinc-oxide nanostructures’. Teaching activity: lectures (18 hours) for the Physics Ph.D. School, on ‘Many Body Perturbation Theory and Time Dependent DFT: Theory and Tools for Electronic-Optical Properties Calculations in Material Science

- awarded by a 2 year fellowship for research activity at the University of the Basque Country, Nano-

Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF), Departamento de Física de Materiales, Unidad de Materiales Centro Mixto CSIC-UPV/EHU Spain, in the framework of the program “Ayudas de especialización para investigadores doctores en la UPV/EHU”.

### **Membership of scientific societies and associations**

- 2024 – present, associated (Associata con incarico di collaborazione) to CNR-INO (Istituto Nazionale di Ottica).
- 2017 – present, GNFM-INdAM
- 2016 – present, SIBPA - Società Italiana di Biofisica Pura ed Applicata
- 2012 – present, AIS3 - Associazione Italiani e Serbi Scienziati e Studiosi
- 2010 – present, ETSF (European Theoretical Spectroscopy Facility) associate member, previously affiliated to the node of UPV/EHU, Spain, and senior ETSF scientist (ETSF Research Team Leader).

### **Supervising Activities**

#### **Ph.D. students:**

- 2022: Supervisor of Marianna Angiolelli, PhD student, XXXVIII ciclo, PhD Program in Bioengineering, Bioscience and Intelligent Systems, UCBM
- 2022: Co-supervisor of Elena Cravero, PhD student, XXXVIII ciclo, PhD Program in Bioengineering, Bioscience and Intelligent Systems, UCBM
- 2021: Co-supervisor of Nicole Luchetti, PhD student, XXXVII ciclo, Ph.D. Program in Science and Engineering for Humans and the Environment, UCBM.
- 2020: Supervisor of Giuseppe Ferrarese, PhD student, XXXVI ciclo, Ph.D. Program in Science and Engineering for Humans and the Environment, UCBM (suspended, March 2022).
- 2018: Co-supervisor of Martina Nicoletti, PhD student, XXXIII ciclo, Ph.D. Program in Science and Engineering for Humans and the Environment, UCBM.

#### **Master and Bachelor students:**

- 2024: Angelo Cassisi, *Master Thesis in Industrial Engineering*, Engineering Department, Campus Bio-Medico University.
- 2024: Alessandro Zirio, *Bachelor Thesis in Industrial Engineering*, Engineering Department, Campus Bio-Medico University.
- 2023: Supervisor of Michelle Viscomi *Bachelor Thesis in Industrial Engineering*, Engineering Department, Campus Bio-Medico University. Thesis title: “Sensori Quantistici Innovativi: gli NV Centers”
- 2022: Co-supervisor of Andrea Sette *Master Thesis in Materials Science and Technology*, Physics & Chemistry Departments, University of Rome Tor Vergata. Thesis title: “An Ab initio study: electronic and optical properties of N-heterocyclic carbenes”
- 2022: Supervisor of Alice Carcone *Bachelor Thesis in Industrial Engineering*, Engineering Department, Campus Bio-Medico University. Thesis title: “Screening methods for early diagnosis of infantile neurodevelopmental deficits in low and middle-income countries: an overview”.
- 2021: Supervisor of Marco Colagiovanni *Bachelor Thesis in Food Science and Human Nutrition*, Department of Sciences and Technologies for Humans and the Environment, Campus Bio-Medico University. Thesis title: “L’applicazione dell’elettroreologia per ridurre il contenuto dei grassi nel cioccolato”.
- 2021: Co-supervisor of Marco Tranchida *Bachelor Thesis in Nursing*, Medicine and Surgery Department, Campus Bio-Medico University (Supervisor Dr. Fabio Mangiacapra). Thesis title: “Microgravità e sistema cardiovascolare: il ruolo dell’assistenza infermieristica nei viaggi spaziali”.
- 2019: Supervisor of Anna Crispino *Bachelor Thesis in Industrial Engineering*, Engineering Department, Campus Bio-Medico University. Thesis title: “Analisi del segnale respiratorio da 4D-CT per l’ottimizzazione del trattamento radioterapico con tecnica Breath-hold.”
- 2017: Supervisor of Margherita Anna Grazia Matarrese *Bachelor Thesis in Industrial Engineering*, Engineering Department, Campus Bio-Medico University. Thesis title: “Computational Study of Structure and Interaction of the Complex HCV IRES – human ribosome”.
- 2017-2018: Supervisor of Riccardo Marrocchio *Master Thesis in Physics*, Physics Department, University of Rome Tor Vergata. Thesis title: “Effective topology of neuronal networks from calcium imaging: extraction and analysis”.
- 2006: Co-supervisor of Stefania D’Agostino *Master Thesis in Physics*, Physics Department, University of Lecce. Thesis title: “Ab initio study of methanethiol adsorbed on Cu(110) metal surface”.

### **Projects and Awards**

- 2023-2025: RNA secondary structures and their relationship with function: application to non-coding RNAs - **RNA2Fun** – funded by **PRIN PNRR 2022** scheme, PI Luca Tesei, Camerino University; <https://bdslab.unicam.it/rna2fun/>  
Role of L. Chiodo: Local unit coordinator (Responsabile di Unita' di Ricerca) at UCBM.  
**Total funding: 239.824 euros**. Local funding 80000 euros. (grant started on 1-12-2023)
- Awarded by the Visiting Professor program University of Cagliari (UNICA) 2009/2010, for 1 month visit, with the project “Ab initio methods for electronic and optical properties in solid state theory, and their application to the study of dye-sensitized zinc-oxide nanostructures”
- Project manager (reference scientist) of the ETSF Training Project of G.Rillo, “Quantum Espresso training” (2014).
- Project manager (reference scientist) of the ETSF user project presented by S. Longo, University of Bari, “Ab initio study of atomic Cs adsorption on Molybdenum surfaces” (2014).
- Project manager (reference scientist) of the ETSF user project, PI R. Tena Zaera, CIDETEC, San Sebastian, Spain, “Hybrid organic/oxide nanosystems for photovoltaic applications: metal-free dyes on ZnO” (2010).
- Project manager (reference scientist) of the ETSF Training Project of A. Iacomino, “Improvement of the theoretical background for the study of the optical properties of TiO<sub>2</sub> nanostructures” (2009).
- Project manager (reference scientist) of the ETSF user project, PI A. Mattoni, CNR, Cagliari, on “Multiscale modeling of organic/metaloxide nanosystems for photovoltaics” (2009).

### **Participation to funded projects**

- 2022-2026: Multiscale quantum bio-imaging and spectroscopy – **MUQUABIS** – Project ID 101070546, funded in the framework of Horizon Europe Framework Programme (HORIZON), under the scheme/call **HORIZON-CL4-2021-DIGITAL-EMERGING-01-21** (Digital and emerging technologies for competitiveness and fit for the green deal), call: Next generation quantum sensing technologies (RIA- Horizon Research and Innovation Action).  
PI: Dr. Nicole Fabbri, INO-CNR. UCBM local coordinator: Prof. Simonetta Filippi.  
Role of L. Chiodo: Co-coordinator of the local research unit.
- 2022-2025: **EBRAINS-Italy** - European Brain ReseArch INfrastructureS-Italy, funded in the framework of PNRR under the scheme Rafforzamento e creazione di Infrastrutture di Ricerca.  
PI: Dr. Michele Migliore, IBF-CNR. URT INO@UCBM local coordinator: Prof. Simonetta Filippi.  
Role of L. Chiodo: Co-coordinator of the local research unit.
- 2022 – 2024 Rome Technopole. UCBM local coordinator: Prof. M. Trombetta; coinvestigator.
- 2020 – 2023: Coordinator of the Ph.D. Industrial Project “Functional Integrated Cancer Receptor (FI-CanceR): ingegnerizzazione di lieviti *Saccharomyces cerevisiae* con recettori funzionali del nematode *Caenorhabditis elegans*, per la realizzazione di un dispositivo bio-medico per la diagnosi precoce del cancro al seno da biofluidi” funded under the program “Regione Lazio PO FSE 2014-2020- Intervento per il rafforzamento della ricerca nel Lazio - incentivi per i dottorati di innovazione per le imprese”.
- 2012, University of Rome La Sapienza Grants, “Methods and applications of classical and quantum molecular dynamics and theory of integrable dynamical systems.”, coinvestigator.
- 2008-2012, ERC StG, “DEDOM Development of Density Functional Theory Methods for organic-metal interaction”, PI F. Della Sala, 1250000 euros, CNR-INFN NNL Lecce, coinvestigator.
- 2007-2009, EC FP6, “SpiDME SPIntronic Devices for Molecular Electronics, coordinator G. Maruccio, CNR-INFN NNL, Lecce, coinvestigator.
- 2005-2007, EC FP6, “SA-NANO Self- Assembly of Shape Controlled Colloidal Nanocrystals”, coordinator Dr. L. Manna, CNR-INFN NNL, Lecce, PostDoc coinvestigator.
- 2004-2007, EC FP6, “Nanoquanta Nanoscale quantum simulations for nanostructures and advanced materials - Nanoquanta Network of Excellence”, Network of Excellence under the NMP3 priority of the European Commission's, coordinator Prof. R. Godby, York, UK, coinvestigator.

### **Participation to computational projects:**

**Principal Investigator (PI) of the European Computational Project** (peer reviewed):

Excited states of metal oxynitrides for Photocatalysis (ECLIPSIS), 2019-2020, 30 M standardised CPU hours, **PRACE** Tier0 Project Access-18th. (Estimated equivalent minimum cost ca. 190000 euro). **Hosts: MARCON2, Budget (standard hours):1 070 000; M100 Host Budget: 575 306**

**Principal Investigator (PI)** of 6 class B (average size) projects at ISCR-CINECA (National HPC Italian Center) (peer reviewed).

PI of 12 class C (small size) projects at ISCR-CINECA (National HPC Italian Center).

Co-investigator in more than 30 national and international Computational Projects (peer reviewed).

### **Publications on Peer Reviewed International Journals**

1. M. Nicoletti, L. Chiodo, A. Loppini, Q. Liu, V. Folli, G. Ruocco, S. Filippi, "Biophysical modeling of the whole-cell dynamics of *C. elegans* motor and interneurons families", *PLoS ONE* 19(3): e0298105 (2024). doi: 10.1371/journal.pone.0298105.
2. M. Nicoletti, N. Luchetti, L. Chiodo, A. Loppini, V. Folli, G. Ruocco, S. Filippi, "Modeling of olfactory transduction in AWCON neuron via coupled electric-calcium dynamics", *Biomolecular Concepts*, 14: 20220035 (2023). doi: 10.1515/bmc-2022-0035.
3. A. Iorio, S. Timr, L. Chiodo, P. Derreumaux, F. Sterpone, "Evolution of Large A $\beta$ 16-22 Aggregates at Atomic Details and Potential of Mean force Associated to Peptide Unbinding and Fragmentation Events", *Proteins* (2023). doi: 10.1002/prot.26500.
4. N. Luchetti, A. Loppini, M. A. G. Matarrese, L. Chiodo, S. Filippi, "Structural Controllability to Unveil Hidden Regulation Mechanisms in Unfolded Protein Response: the Role of Network Models", *Physica A* (2023). doi: 10.1016/j.physa.2023.128671.
5. M. Lauricella, L. Chiodo, F. Bonaccorso, M. Durve, A. Montessori, A. Tiribocchi, A. Loppini, S. Filippi, S. Succi, "Multiscale Hybrid Modeling of Proteins in Solvent: SARS-CoV2 Spike Protein as test case for Lattice Boltzmann - All Atom Molecular Dynamics Coupling", *Communications in Computational Physics* 33 (1), 57-76 (2023). doi: 10.4208/cicp.OA-2022-0046.
6. M. A. G. Matarrese, A. Loppini, M. Nicoletti, S. Filippi, L. Chiodo, "Assessment of tools for RNA secondary structure prediction and extraction: a final-user perspective", *Journal of Biomolecular Structure & Dynamics* 41 (14), 6917-6936 (2023). doi: 10.1080/07391102.2022.2116110.
7. G. Cottone, L. Chiodo, L. Maragliano, M.-R. Popoff, C. Razetti-Escargueil, E. Lemichez, T.E. Malliavin, "*In silico* conformational features of botulinum toxins A1 and E1 according to intraluminal acidification", *Toxins* 14(9), 644 (2022). doi: 10.3390/toxins14090644.
8. C. Guardiani, F. Cecconi, L. Chiodo, G. Cottone, P. Malgaretti, L. Maragliano, M. L. Barabash, G. Camisasca, M. Ceccarelli, B. Corry, R. Roth, A. Giacomello, B. Roux, "Computational methods and theory for ion channel research", *Advances in Physics: X* 7, 2080587 (2022). doi: 10.1080/23746149.2022.2080587.
9. S. Ghirga, L. Chiodo, R. Marrocchio, J. G. Orlandi, A. Loppini, "Inferring excitatory and inhibitory connections in neuronal networks", *Entropy* 23(9), 1185 (2021). doi: 10.3390/e23091185.
10. D. Caprini, S. Schwartz, E. Lanza, E. Milanetti, V. Lucente, G. Ferrarese, L. Chiodo, M. Nicoletti, V. Folli, "A shearless microfluidic device detects a role in mechanosensitivity for AWCON neuron in *C. elegans*", *Advanced Biology* 2100927 (2021). doi: 10.1002/adbi.202100927.
11. G. Cottone, L. Chiodo, L. Maragliano, "Thermodynamics and kinetics of ion translocation in the human wild-type and E-1'A  $\alpha$ 7 nicotinic receptor", *Nuovo Cimento C - Colloquia and Communications in Physics*, Società Italiana di Fisica, 44, 4-5, 127 (2021). doi: 10.1393/ncc/i2021-21127-1.
12. M. Nicoletti, L. Chiodo, A. Loppini, "Biophysics and modeling of mechanotransduction in neurons: a review", Special Issue: "Mathematical Modeling in Biomechanics and Mechanobiology", *Mathematics* 9, 323 (2021). doi: 10.3390/math9040323
13. G. Cottone, L. Chiodo, L. Maragliano, "Thermodynamics and kinetics of ion permeation in wild-type and mutated open active conformation of the human  $\alpha$ 7 nicotinic receptor", *J. Chem. Inf. Model.* 60, 10, 5045–5056 (2020). doi: 10.1021/acs.jcim.0c00549.
14. A. Patra, S. Jana, L. A. Constantin, L. Chiodo, P. Samal, "Improved transition metal surface energies from a generalized gradient approximation developed for quasi two-dimensional quantum systems", *J. Chem. Phys.* 152, 151101 (2020). doi: 10.1063/1.5145367
15. D. Salerno, L. Chiodo, V. Alfano, O. Floriot, G. Cottone, A. Paturel, M. Pallocca, M.-L. Plissonnier, S. Jeddari, L. Belloni, M. B. Zeisel, M. Levrero, F. Guerrieri, "Hepatitis B protein HBx binds the DLEU2 lncRNA to sustain cccDNA and host cancer-related gene transcription", *Gut* 69, 2016-2024 (2020). doi: 10.1136/gutjnl-2019-319637.
16. M. Lauricella, L. Chiodo, G. Ciccotti, A. Albinati, "*Ab initio* accelerated molecular dynamics study of the hydride ligands in the ruthenium complex: Ru(H<sub>2</sub>)<sub>2</sub>H<sub>2</sub>(P(C<sub>5</sub>H<sub>9</sub>)<sub>3</sub>)<sub>2</sub>", *Phys Chem Chem Phys* 21, 25247-25257 (2019). doi: 10.1039/C9CP03776D
17. A. Loppini, L. Chiodo, "Biophysical modeling of  $\beta$ -cells networks: realistic architectures and heterogeneity effects", *Biophys. Chem.* 254, 106247 (2019). doi: 10.1016/j.bpc.2019.106247
18. M. Nicoletti, A. Loppini, L. Chiodo, V. Folli, G. Ruocco, S. Filippi, "Biophysical modeling of *C.*

- C. elegans* neurons: single ion currents and whole-cell dynamics of AWC<sup>on</sup> and RMD”, PLoS ONE 14(7): e0218738 (2019). doi: 10.1371/journal.pone.0218738;
19. L. Chiodo, “Two-dimensional innovative materials for photovoltaics”, Current Opinion in Green and Sustainable Chemistry 17, 49-56 (2019). doi: 10.1016/j.cogsc.2019.04.004.
  20. L. Chiodo, T. E. Malliavin, S. Giuffrida, L. Maragliano, G. Cottone, “Closed-locked and apo-resting state structures of the human  $\alpha 7$  nicotinic receptor: a computational study”, J. Chem. Inf. Model. 58, 2278 (2018). doi: 10.1021/acs.jcim.8b00412.
  21. L. Chiodo, T. E. Malliavin, L. Maragliano, G. Cottone, “A possible desensitized state conformation of the human  $\alpha 7$  nicotinic receptor: a molecular dynamics study”, Biophys. Chem. 229, 99-109 (2017). doi: 10.1016/j.bpc.2017.06.010.
  22. E. Baldini, A. Dominguez, L. Chiodo, E. Sheveleva, M. Yazdi-Rizi, C. Bernhard, A. Rubio, M. Chergui., “Anomalous exciton temperature dependence in rutile TiO<sub>2</sub>”, Phys. Rev. B 96, 041204(R) (2017). doi: 10.1103/PhysRevB.96.041204.
  23. E. Baldini, L. Chiodo, A. Dominguez, M. Palummo, S. Moser, M. Yazdi-Rizi, G. Auböck, B. Mallett, H. Berger, A. Magrez, C. Bernhard, M. Grioni, A. Rubio, M. Chergui, “Strongly bound excitons in anatase TiO<sub>2</sub> single crystals and nanoparticles”, Nat. Comm. 8, 13 (2017). doi:10.1038/s41467-017-00016-6.
  24. Y. Zhihua, P. E. Trevisanutto, L. Chiodo, I. Santoso, A. R. Barman, T. C. Asmara, S. Dhar, A. Terentjev, F. Della Sala, V. Olevano, T. Venkatesan, A. Rusydi, “Emerging giant resonant exciton induced by Ta substitution in anatase TiO<sub>2</sub>: A tunable correlation effect”, Phys. Rev. B 93, 205118 (2016). doi: 10.1103/PhysRevB.93.205118.
  25. L. Chiodo, T. E. Malliavin, L. Maragliano, G. Cottone, G. Ciccotti, “A structural model of the human  $\alpha 7$  nicotinic receptor in an open conformation”, Plos One 10 (7), e0133011 (2015). OA. doi: 10.1371/journal.pone.0133011
  26. A. Damone, A. Panarese, C. Coppola, J. Jansky, C. Coletti, L. Chiodo, G. Serianni, V. Antoni, S. Longo, “Theoretical determination of the microstructure of Cs covering of Mo in negative ion sources for nuclear fusion applications”, Plasma Phys. Control. Fusion 57, 035005 (2015).
  27. F. Gentile, M. Monteferrante, L. Chiodo, A. Toma, M. L. Coluccio, G. Ciccotti, E. Di Fabrizio, “Electroless formation of silver nanoaggregates: an experimental and molecular dynamics approach”, Mol. Phys. 112 (9-10), 1375-1388 (2014).
  28. 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).
  29. 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).
  30. G. Roma, L. Chiodo, “Selenium adsorption on Mo(110): a first principles investigation”, Phys. Rev. B 87, 245420 (2013)
  31. 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).
  32. M. Palummo, G. Giorgi, L. Chiodo, A. Rubio, and K. Yamashita “The nature of radiative transitions in TiO<sub>2</sub>-based nanosheets”, J. Phys. Chem. C 116, 18495- 18503 (2012).
  33. 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).
  34. L. Chiodo, L. A. Constantin, E. Fabiano, and F. Della Sala, “Nonuniform scaling applied to surface energies of transition metals”, Phys. Rev. Lett. 108, 126402 (2012).
  35. L. Chiodo, M. Salazar, A. H. Romero, S. Laricchia, F. Della Sala, and A. Rubio, “Structure, electronic and optical properties of TiO<sub>2</sub> atomic clusters: an ab initio study”, J. Chem. Phys. 135, 244704 (2011) (doi: 10.1063/1.3668085).
  36. 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).
  37. 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).
  38. 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 TiO<sub>2</sub> crystalline phases”, Phys. Rev. B 82, 045207 (2010).
  39. A. Ruocco, L. Chiodo, M. Sforzini, M. Palummo, P. Monachesi, G. Stefani, “Experimental and theoretical investigation of the pyrrole/Al(100) interface”, J. Phys. Chem. A 113, 15193–15197 (2009).
  40. L. Chiodo, F. Della Sala, T. Pellegrino, R. Cingolani, L. Manna, “An ab initio study of the magnetic-metallic CoPt<sub>3</sub>-Au interfaces”, J. Phys.: Condens. Matt. 21 015001 (2009).
  41. V. Arima, R. I. R. Blyth, F. Matino, L. Chiodo, F. Della Sala, J. Thompson, T. Regier, R. Del Sole,

- G. Mele, G. Vasapollo, R. Cingolani and R. Rinaldi, "Zinc porphyrin - driven assembly of gold nanofingers", *Small* 4 (4), 497-506 (2008).
42. L. Carbone, C. Nobile, M. De Giorgi, F. Della Sala, G. Morello, P.P. Pompa, M. Hytch, E. Snoeck, A. Fiore, I. R. Franchini, M. Nadasan, A. F. Silvestre, L. Chiodo, S. Kudera, R. Cingolani, R. Krahné and L. Manna, "Synthesis and micrometer-scale assembly of colloidal CdSe/CdS nanorods prepared by a seeded growth approach", *Nano Lett.* 7, 2942 (2007).
  43. S. D'Agostino, L. Chiodo, F. Della Sala, R. Cingolani, R. Rinaldi, "Ab initio structural and electronic analysis of CH<sub>3</sub>SH self-assembled on a Cu(110) substrate", *Phys. Rev. B* 75, 195444 (2007).
  44. D. Fragouli, T. N. Kitsopoulos, L. Chiodo, F. Della Sala, R. Cingolani, S. G. Ray, R. Naaman, "Imaging photoelectron transmission through self-assembled monolayers: the work function of alkanethiols coated gold", *Langmuir* 23(11), 6156 (2007).
  45. M. G. Betti, F. Bussolotti, L. Chiodo, P. Monachesi, C. Mariani, "Anchoring sulphur-headgroup organic molecules at Cu(100): tailoring the interface electronic states", *Surf. Sci.* 601 (13), 2580-2583 (2007).
  46. L. Chiodo, P. Monachesi, "Role of coverage on the electronic properties of sulfur chemisorbed on Cu(100): Ab initio calculations", *Phys. Rev. B* 75, 075404 (2007).
  47. P. Monachesi, L. Chiodo, "Optical response of Copper surface to Carbon monoxide deposition", *Phys. Rev. Lett.* 93, 116102 (2004).
  48. P. Monachesi, L. Chiodo, R. Del Sole, "Ab initio characterization of surface states at the S/Cu(100) interface", *Phys. Rev. B* 69, 165404 (2004).
  49. C. Baldacchini, L. Chiodo, F. Allegretti, C. Mariani, M.G. Betti, P. Monachesi, R. Del Sole, "Cu(100) surface: High resolution experimental and theoretical band mapping", *Phys. Rev. B* 68, 195109 (2003).

#### Book chapters and contributions in volumes

50. M. Lauricella, L. Chiodo, F. Bonaccorso, M. Durve, A. Montessori, A. Tiribocchi, A. Loppini, S. Filippi, S. Succi, "Computational Investigation of Wild-Type and Alpha Variant SARS-CoV-2 Spike Protein by Multiscale Modeling, in "CRESCO Annual Report 2021", Edizioni ENEA (2021). Contributo in monografia. ISBN:
51. M. Lauricella, L. Chiodo, F. Bonaccorso, M. Durve, A. Montessori, A. Tiribocchi, A. Loppini, S. Filippi, S. Succi, "Multiscale Modeling of Wild-Type and Alpha Variant SARS-CoV-2 Spike Protein", in "ENEA CRESCO in the fight against COVID-19", Editor F. Iannone, Edizioni ENEA (2021). Contributo in monografia. ISBN:978-88-8286-414-6.
52. G. Cottone, L. Chiodo, T. E. Malliavin, L. Maragliano, "A full atomistic computational study of the inactive states of the human  $\alpha 7$  nicotinic receptor", in Cineca HPC Report 2017.
53. L. Chiodo, G. Giorgi, M. Palummo, "Electronic and Optical Properties of Oxides Nanostructures by first-principles Approaches", in *Encyclopedia of Nanotechnology*, edited by Bharat Bhushan, Springer (2015). ISBN 978-94-017-9779-5 ISBN 978-94-017-9780-1 (eBook) ISBN 978-94-017-9781-8 (print and electronic bundle). doi: 10.1007/978-94-017-9780-1\_100933.
54. L. Chiodo, T. E. Malliavin, L. Maragliano, G. Cottone, G. Ciccotti, "Large scale motions in models of human nicotinic receptors", in Cineca HPC Report 2014.
55. L. Chiodo, J. M. García-Lastra, D. J. Mowbray, A. Iacomino, A. Rubio, "Tailoring electronic and optical properties of TiO<sub>2</sub>: nanostructuring, doping and molecular-oxide interactions", in "Computational Studies of New Materials II: From Nanostructures to Bulk Energy Conversion Materials", edited by T. F. George, D. Jelski, R. R. Letfullin and Dr. G. Zhang, pp. 301-329, World Scientific (2011). doi: 10.1142/9789814287197\_0012
56. L. Chiodo, A. Iacomino, M. Palummo, A. Rubio, "Titania nanostructures electronic and optical response", in "Handbook of Functional Nanomaterials, Vol. 2, edited by Mahmood Aliofkhaezrai, Series: Nanotechnology Science and Technology, Nova Science Publishers, Ltd. (New York – USA) (2014). ISBN: 978-1-62948-168-5.

#### Conference Papers (Peer reviewed)

57. N. Luchetti, L. Chiodo, A. Loppini, S. Filippi "Multiscale Evaluation of Electrophysiological Properties of Ion Channels: from Atomistic Description to Hodgkin-Huxley Models", 2022 IEEE International Workshop on Metrology for Industry 4.0 & IoT, 109 – 104 (2022). Conference paper. doi: 10.1109/MetroInd4.0IoT54413.2022.9831546
58. M. Nicoletti, A. Loppini, L. Chiodo, V. Folli, G. Ruocco, S. Filippi, "Mathematical modeling of the Caenorhabditis elegans RMD motor neurons", 11th Conference of the European Study Group on Cardiovascular Oscillations (ESGCO), 2020. Proceedings doi: 10.1109/ESGCO49734.2020.9158182.
59. M. Nicoletti, A. Loppini, L. Chiodo, V. Folli, G. Ruocco, S. Filippi, "AWC C. elegans neuron: a biological sensor model", 2020 IEEE International Workshop on Metrology for Industry 4.0 & IoT,

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60. G. Roma, L. Chiodo, J. Kiss, "Adsorption of Se, Na, and O on the Mo(110) surface: Modeling atomic mechanisms at the back contact of thin film chalcopyrite solar cells", Photovoltaic Specialists Conference (PVSC), 2013 IEEE 39th, pp 3300-3303. Doi: 10.1109/PVSC.2013.6745156.
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  62. L. Chiodo, A. Massaro, R. Cingolani, A. Romero, A. Rubio, "Characterization of TiO<sub>2</sub> atomic crystals for nanocomposite materials oriented to optoelectronics", 2011 Numerical Simulation of Optoelectronic Devices, IEEE, Conference Paper, doi: 10.1109/NUSOD.2011.6041192
  63. L. Chiodo, M. Bruno, M. Palummo, P. Monachesi, "First-principles optical spectra of low dimensional systems", *Phys. Stat. Sol. (b)* **242**, 3032 (2005). doi: 10.1002/pssb.200562242.
  64. P. Monachesi, L. Chiodo, F. Bussolotti, M. G. Betti, C. Mariani, "Anchoring of Organic Molecules on Cu(001) Surface through S-headgroup", *Mater. Res. Soc. Symp. Proc. Vol. 872, J2.2.1* (2005). doi: 10.1016/j.susc.2006.11.051.

#### Conference Abstracts (indexed)

65. E. Baldini, A. Dominguez, T. Palmieri, L. Chiodo, M. Palummo, P. Ruello, A. Rubio, M. Chergui, "Discovery and room-temperature ultrafast manipulation of strongly bound excitons in anatase TiO<sub>2</sub>", Abstract of papers of the American Chemical Society, Vol. 256, Editor Amer. Chem. Soc. (2018).
66. F. Guerrieri, D Salerno, L. Chiodo, G. Cottone, M. Pallocca, O. Floriot, M. Levrero, "HBx/DLEU2/EZH2 co-regulation of host genes expression in HCC", *Journal of Hepatology* **68**, S687-S688 (2018). doi: 10.1016/S0168-8278(18)31634-9, WOS:000461068603177
67. F. Guerrieri, L. Chiodo, D Salerno, O Floriot, S Jeddari, G Ruocco, M. Levrero, "The binding of the DLEU2 lncRNA to HBx and the cccDNA affects viral chromatin transcription in HBV infected cells", *Hepatology* **64** (1 SUPP), 315A-316A, n.633 (2016)
68. F. Guerrieri, L. Chiodo, D Salerno, S Jeddari, G Ruocco, M Levrero, "The HBX-DLEU2 LNCRNA complex regulates transcription from the HBV CcDNA and from cellular genes in cis and in trans", *Journal of Hepatology* **64** (2), S388 (2016). doi: 10.1016/S0168-8278(16)00600-0.
69. F. Guerrieri, L Chiodo, D Salerno, S Jeddari, G Ruocco, M. Levrero, "The HBx-DLEU2 lncRNA complex regulates transcription from cellular genes and the HBV cccDNA", *Hepatology* **62**, 293A (2015)
70. F. Guerrieri, L Chiodo, S Jeddari, D D'Andrea, G Ruocco, A Tramontano, M Levrero, "HBx-DLEU2 lncRNA complex affects transcription of new target promoters", *Journal of Hepatology* **62**, issue S1, S514-S515 (2015). doi: 10.1016/S0168-8278(15)31537-3,
71. F. Guerrieri, L. Chiodo, S.Jeddari, D. D'Andrea, A. Tramontano, G. Ruocco, M. Levrero, "HBx-DLEU2 lncRNA complex affects transcription of new target promoters", *Digestive and Liver Disease* **47**, e30 (2015). Abstracts of the 48th A.I.S.F. – Italian Association for the Study of the Liver – Annual Meeting 2015, Doi: <https://doi.org/10.1016/j.dld.2015.01.068>,

#### Papers under review

1. A. Crispino, M. Nicoletti, A. Loppini, A. Gizzi, L. Chiodo, C. Cherubini, S. Filippi, "Magnetic Signature of Thermo-Electric Cardiac Dynamics (submitted, July 2024). arXiv:2406.20084
2. \* N. Luchetti, K. M. Smith, M.A.G. Matarrese, A. Loppini, L. Chiodo, S. Filippi, A statistical mechanics investigation of Unfolded Protein Response across species (submitted, August 2024). arXiv:2407.12464
3. M. Angiolelli, D. Depannemaecker, H. Agouram, J. Régis, R. Carron, M. Woodman, L. Chiodo, P. Triebkorn, A. Ziaemehr, M. Hashemi, A. Eusebio, V. Jirsa, P. Sorrentino, "The Virtual Parkinsonian Patient" (submitted, August 2024). 10.1101/2024.07.08.24309856
4. M. Angiolelli, S. Scarpetta, P. Sorrentino, E. Troisi Lopez, M. Quarantelli, C. Granata, G. Sorrentino, V. Palmieri, G. Messuti, M. Stefano, S. Filippi, C. Cherubini, A. Loppini, and L. Chiodo, "Criticality explains structure-function relationships in the human brain", (submitted, August 2024). 10.1101/2024.07.15.603226
5. M. Angiolelli, S. Scarpetta, P. Sorrentino, E. Troisi Lopez, M. Quarantelli, C. Granata, G. Sorrentino, G. Messuti, S. Filippi, A. Loppini, L. Chiodo, and C. Cherubini, "Exploring criticality in brain dynamics through Avalanche Configurations Matrix and its spectrum", (submitted, July 2024)

### **Invited Talks**

- 8-12 May 2017, Workshop on Spectroscopy and Dynamics of Photoinduced Electronic Excitations, ICTP, Trieste, Italy. Talk: "Anomalous excitons in titanium dioxide"
- 23-27 June 2014, "Nanostructured Zinc Oxide and related materials", Cecam Workshop, Bremen Center for Computational Materials Science, Bremen, Germany. Talk: "Optical properties of inorganic nanostructures: low dimensionality and confinement effects"

### **Conferences Organization**

- 7-9 June 2022, IEEE International Workshop on Metrology for Industry 4.0 and IoT -MetroInd4.0&IoT, Trento, Italy. Co-organizer of the Special session on "The frontiers of sensing: quantum and biosensors"
- 24-28 August 2021, DynamicsDays2020–XL, Nice, France. Co-organizer of minisymposium on "Neuronal Dynamics: from single cell up to large-scale networks".
- 3-5 May 2006, Nanoquanta Young Researchers' Meeting, Rome, Italy. Co-organizer.

### **Invited Seminars**

- 2 February 2024, Dipartimento di Matematica e Fisica, Università degli Studi Roma Tre. Physics Colloquia: "*Computational study of non-coding RNA structures and their interaction with proteins*".
- 4 June 2019, Pasteur Institute, Paris, France. Talk: "*Open-active and closed-inactive states of the human  $\alpha 7$  nicotinic receptor: a molecular dynamics perspective*".
- 20 April 2015, Institute for Advanced Simulations (IAS), Computational Biomedicine (IAS-5 / INM-9), Forschungszentrum Jülich, Germany. Talk: "*Transition metals oxides, from extended systems to nanostructures: ab initio electronic and optical properties*".
- 17 February 2015, IPCMS, CNRS, Strasbourg, France. Talk: "*Electronic and optical properties of transition metals oxides: from extended systems to nanostructures*".
- 24 October 2007, University of L'Aquila, Italy. Talk: "*Thiol adsorption effects on copper and gold work function*".
- 3 May 2005, NNL of CNR-INFM, Lecce, Italy. Talk: "*Ab initio calculations of electronic and optical properties: theory and applications*".