Curriculum vitae

Full name: Nicola Seriani
Date of birth: 19^{th} March 1977
Place of birth: Trieste (Italy)
Nationality: Italian
Phone: +39 040 2240 279 (w)

Address: Strada Costiera 11
34151 Trieste
Italy

Email: nseriani@ictp.it

Employment

- 2024- Research scientist at the Condensed Matter and Statistical Physics Section at the Abdus Salam International Centre for Theoretical Physics in Trieste.
- 2018-2024 Associate research scientist at the Condensed Matter and Statistical Physics Section at the Abdus Salam International Centre for Theoretical Physics in Trieste.
- 2011-2018 Long-term visiting scientist at the Condensed Matter and Statistical Physics Section at the Abdus Salam International Centre for Theoretical Physics in Trieste.
- 2009-2011 Postdoc fellow at the Condensed Matter and Statistical Physics Section at the Abdus Salam International Centre for Theoretical Physics in Trieste.
- 2006-2009 Employed as scientist at the Computational Materials Physics Group, University of Vienna (group of J. Hafner and G. Kresse).
- 2002-2006 Employed as scientist at the Institute for Materials Science, Dresden University of Technology (Germany). Quantum modelling of platinum oxides and catalytic processes. In August 2003 and October 2004 guest scientist at TCM, Cavendish Laboratory, University of Cambridge.
- 2001-2002 Compulsory social service at the old people's home ITIS in Trieste (Italy).

Education

- 2002-2006 Ph.D. student of materials science at the Dresden University of Technology (Germany). Ph.D. thesis entitled "First-principles simulations of the oxidation of methane and CO on platinum oxide surfaces and thin films" under the supervision of Prof. W. Pompe. Courses taken: technical thermodynamics, materials science, biomolecular nanotechnology and metal physics. Final mark: summa cum laude.
- 1996-2001 Physics student at the University of Trieste (Italy). Graduated with full marks (110/110 cum laude). Thesis entitled: "Confinement effects for a quantum wire model" (in Italian), under the supervision of Prof. G. Senatore; small thesis entitled: "Results of the K2K experiment on neutrino oscillations" (in Italian), under the supervision of Prof. G. Giannini. Courses taken in the final year of study: solid state physics, quantum theory of matter, elementary particles physics and field theory.

- 1991-1996 High-school "G. Oberdan", Trieste (Italy). Full marks (60/60) in the final examination. Participation in the Physics Olympiads (placed in the first twenty at national level), Mathematics Olympiads (placed in the first fifty at national level) and Mathematical Games (placed seventh at national level in my age group).

Computational grants

- ISCRA 2017/2018 Type B (1,000,000 CPU hours), N. Seriani (PI), E. Poli, K. Ulman, KINCAT - Kinetics of charge transfer during photocatalytic water splitting at the hematite/water interface from constrained density functional theory simulations
- PRACE Tier-0 2016/2017 (28,000,000 CPU hours), S. Piccinin (PI), N. Seriani, M. Farnesi Camellone, FESTAWOX - Free energy surface of proton coupled electron transfers in water oxidation: the case of hematite
- ISCRA 2013/2014 Type B (2,600,000 CPU hours), R. Gebauer (PI), N. Seriani, M.-T. Nguyen, I. Girotto, Photoinduced water splitting on defective hematite surfaces
- ISCRA 2012/2013 Type B (5,000,000 CPU hours), N. Seriani (PI), R. Gebauer, Y. Crespo, I. Girotto, First-principles simulations of materials for the photocatalytic conversion of water and carbon dioxide into hydrocarbons
- ISCRA 2011/2012 Type C (50,000 CPU hours), N. Seriani (PI), C. Pinilla, Y. Crespo, Catalysts for the production of solar fuels: the case of copper
- ISCRA 2011/2012 Type B (280,000 CPU hours), R. Gebauer (PI), N. Seriani, M.-T. Nguyen, Hematite for solar energy applications

Publications

BOOK: N. Seriani, Platinum Oxides in Heterogenous Catalysis; Publisher: VDM Verlag Dr. Mueller e.K. (July 8, 2008); ISBN-10: 3639055268; ISBN-13: 978-3639055269

ARTICLES:

90. Nicola Seriani, Paola Delcompare-Rodriguez, Dhanshree Pandey, Abhishek Kumar Adak, Vikram Mahamiya, Carlos Pinilla, and Hala J. El-Khozondar, "Quantitative analysis of the synergy of doping and nanostructuring of oxide photocatalysts", Materials 17, 3460 (2024)

89. Mohammad Ali Mohebpour, Sahar Izadi Vishkayi, Valerio Vitale, Nicola Seriani, Meysam Bagheri Tagani, "Origin and properties of the flat band in monolayer NbOCl2", Physical Review B 110, 035429 (2024)

88. Mohamed El-Kinawy, Nicola Seriani, Fathy Abdel-Wahab, Nabil El-Faramawy, "DFT study of the role and possible contribution of defects to lithium metasilicate luminescence", Journal of Solid State Chemistry 338, 124890 (2024)

87. Kossi Kety, Tsogbadrakh Namsrai, Huma Nawaz, Samare Rostami, Nicola Seriani, "Amorphous MoS2 from a machine learning inter-atomic potential", Journal of Chemical Physics 160, 204709 (2024); JCP Editor's Pick

86. Paolo Lazzari, Nicola Seriani, "Universality of two-dimensional cellular automata - Deterministic models of growth", Chaos, Solitons & Fractals 185, 114997 (2024)

85. Volker Blum, Ryoji Asahi, Jochen Autschbach, Christoph Bannwarth, H. Bernhard Schlegel, Gustav Bihlmayer, Stefan Blugel, Lori A. Burns, T. Daniel Crawford, William Dawson, Wibe Albert de Jong, Claudia Draxl, Claudia Filippi, Luigi Genovese, Paolo Giannozzi, Niranjan Govind, Sharon Hammes-Schiffer, Jeff R. Hammond, Ben Hourahine, Anubhav Jain, Yosuke Kanai, Paul R. C. Kent, Ask Hjorth Larsen, Susi Lehtola, Xiaosong Li, Roland Lindh, Nancy Makri, Satoshi Maeda, Jonathan Moussa, Takahito Nakajima, Jessica A. Nash, Micael J. T. Oliveir, Pansy D. Patel, Giovanni Pizzi, Geoffrey Pourtois, Benjamin P. Pritchard, Eran Rabani, Markus Reiher, Lucia Reining, Xinguo Ren, Mariana Rossi, Nicola Seriani, Lyudmila V. Slipchenko, Alex J. W. Thom, Edward F. Valeev, Benoit Van Troeye, Lucas Visscher, Vojtech Vlcek, Hans-Joachim Werner, David B. Williams-Young, and Theresa L. Windus, "Roadmap on software for electronic structure-based simulations in chemistry and materials", Electronic structure, accepted (05/2024)

84. Hua-Jian Tan, Rutong Si, Nicola Seriani, Xiao-Lin Wei, Wen-Jin Yin, and Ralph Gebauer, "How spin state and oxidation number of transition metal atoms determine molecular adsorption: a first-principles case study for NH_3", Physical Chemistry Chemical Physics 26, 7688 (2024)

83. Yun-Bo Li, Rutong Si, Bo Wen, Xiao-Lin Wei, Nicola Seriani, Wen-Jin Yin, and Ralph Gebauer, "The Role of Water Molecules on Polaron Behavior at Rutile (110) Surface: a Constrained Density Functional Theory Study", The Journal of Physical Chemistry Letters 15, 1019 (2024)

82. Gonzalo Diaz Miron, Jonathan Semelak, Luca Grisanti, Alex Rodriguez, Irene Conti, Martina Stella, Nicola Seriani, Ivan Rivalta, Marco Garavelli, Dario Estrin, Mariano C. Gonzalez Lebrero, Ali Hassanali, and Uriel N. Morzan, "The "Carbonyl-Lock" Mechanism Underlying Non-Aromatic Fluorescence in Biological Matter", Nature Communications 14, 7325 (2023)

81. Dawei Deng, Rutong Si, Bo Wen, Nicola Seriani, Xiao-Lin Wei, Wen-Jin Yin, Ralph Gebauer, "Self-doped p-n junctions with high carrier concentration in 2D GaN/MoSSe heterostructures: a first-principles study", Journal of Materials Chemistry A 11, 22360 (2023)

80. Luis A. Alcala-Varilla, Rafael E. Ponnefz-Durango, Nicola Seriani, Eduard Araujo-Lopez, and Javier A. Montoya, "A DFT + U Study on the Stability of Small CuN Clusters (N = 3-6 Atoms): Calculation of Phonon Frequencies", Condens. Matter 8, 81 (2023)

79. Mesfin Diro Chaka, Chernet Amente Geffe, Alex Rodriguez, Nicola Seriani, Qin Wu, Yedilfana Setarge Mekonnen, "A Molecular Graph Attention Networks (MolGAT) Model to Predict Redox Potential of Organic Materials and the Virtual Screening of Redox-Active Species", ACS Omega 8, 24268 (2023)

78. Tamadhur Alaa Hussein, Warood Kream Alaarage, Heider A. Abdulhussein, Nicola Seriani, Abbas H. Abo Nasria, "Ga-doped AlN monolayer nano-sheets as promising materials for environmental sensing applications", Computational and Theoretical Chemistry 1223, 114086 (2023)

77. Mohamed El-Kinawy, Fathy Abdel-Wahab, Nicola Seriani, Nabil El-Faramawy, "DFT study of the role of point and complex defects on luminescence, electronic, and thermodynamic properties of LiF:Mg", Materials Research Bulletin 158, 112044 (2023)

76. Samare Rostami, Nicola Seriani, Ralph Gebauer, "Hematite surfaces: band bending and local electronic states", Physical Review Materials 6, 104604 (2022)

75. Nicola Seriani, "An ab-initio study of clusters as building blocks for crystals: from Prussian blue analogues to hybrid perovskites", Physica Status Solidi B 2200045, (2022)

74. Gebremedhn Gebreyesus, Prosper Ngabonziza, Jonah Nagura, Nicola Seriani, Omololu Akin-Ojo, Richard M. Martin, "Electronic Structure and Magnetism of the Three-layered Ruthenate Sr4Ru3O10", Physical Review B 105, 165119 (2022)

73. Elham Moharramzadeh Goliaei, Nicola Seriani, "N2O Decomposition on Ti3O6 Deposited on Anatase(101) from the First-Principles Calculations: The Role of Oxygen Vacancy", Applied Surface Science 579, 152215 (2022)

72. Paola A. Delcompare-Rodriguez, Nicola Seriani, "Ultrathin space charge layer in hematite photoelectrodes: a theoretical investigation", Journal of Chemical Physics 155, 114701 (2021)

71. Samare Rostami, Nicola Seriani, S. Alireza Ghasemi, Ralph Gebauer, "Accurate and flexible neural-network interatomic potential for mixed materials: TixZr1-xO2 from bulk to clusters and nanoparticles", Physical Review Materials 5, 063605 (2021)

70. Deobrat Singh, Sanjeev K. Gupta, Nicola Seriani, Igor Lukacevic, Yogesh Sonvane, P. N. Gajjar, Rajeev Ahuja, "Mechanism of formaldehyde and formic acid formation on (101)-TiO2@Cu4 system through CO2 hydrogenation", Sustainable Energy & Fuels 5, 564 (2021)

69. Jyotirmoy Deb, Nicola Seriani, Utpal Sarkar, "Ultrahigh carrier mobility of penta-

graphene: A first-principle study", Physica E: Low-dimensional Systems and Nanostructures 127, 114507 (2021)

68. Francesco Armillotta, Alex Pividori, Matus Stredansky, N. Seriani, E. Vesselli, "Dioxygen at biomimetic single metal-atom sites: stabilization or activation? The case of CoTPyP/Au(111)", Topics in Catalysis 63, 1585 (2020)

67. Henry Andres Cortes, Maria A. Barral, N. Seriani, Horacio R. Corti, Veronica L. Vildosola, "Revealing the Li2O2 nucleation mechanisms on CeO2 catalysts for lithium-oxygen batteries", ChemCatChem 12, 4132 (2020)

66. Nandhakumar Velankanni, N. Seriani, Ralph Gebauer, "DFT Insights into Electrocatalytic CO2 Reduction to Methanol on alpha-Fe2O3(0001) Surfaces", Physical Chemistry Chemical Physics 22, 10819 (2020)

65. Alam Khorsed, N. Seriani, Prasenjit Sen, "Catalytic properties of alpha-MnO2 for Li-air battery cathodes: a density functional investigation", Physical Chemistry Chemical Physics 22, 9233 (2020)

64. Catherine Paschal, Alexander Pogrebnoi, Tatiana Pogrebnaya, N. Seriani, "Methylammonium tin iodide perovskite: structural, electronic and thermodynamic properties by a DFT study with different exchange-correlation functionals", SN Applied Sciences 2, 718 (2020)

63. Wala Elsayed, Sahar Abdalla, N. Seriani, "Quasi-particle and Optical Properties of Hydrogen Titanate and Its Defective Systems: an Investigation by DFT+U, GW, and BSE", Physica Status Solidi B: Basic Solid State Physics 1900054 (2019)

62. Geradius Deogratias, N. Seriani, Tatiana Pogrebnaya, Alexander Pogrebnoi, "Tuning optoelectronic properties of triphenylamine based dyes through variation of pi-conjugated units and anchoring groups: A DFT/TD-DFT investigation", Journal of Molecular Graphics and Modelling 94, 107480 (2019)

61. L. Alcala Varilla, N. Seriani, J. Montoya, "Molecular adsorption and dissociation of CO2 on TiO2 anatase (001) activated by oxygen vacancies", Journal of Molecular Modeling 25, 231 (2019)

60. E. Shomali, I. Abdolhosseini Sarsari, F. Tabatabaei, M. R. Mosaferi, N. Seriani, "Graphyne as the anode material of magnesium-ion batteries: ab initio study", Computational Materials Science 163, 315 (2019)

59. Alam Khorsed, N. Seriani, Prasenjit Sen, "alpha-MnO2 under pressure: possible route to delta-MnO2", Materials Research Express 6, 076108 (2019)

58. M. Corva, F. Mohamed, E. Tomsic, M. Rinaldi, C. Cepek, N. Seriani, M. Peressi, E. Vesselli, "Learning from Nature: Charge Transfer and Carbon Dioxide Activation at Single, Biomimetic Fe Sites in Tetrapyrroles on Graphene", The Journal of Physical Chemistry C 123, 3916 (2019)

57. E. M. Goliaei, N. Seriani, "Structure and electronic properties of small silver-gold clusters on titania photocatalysts: an investigation with density functional theory", The Journal of Physical Chemistry C 123, 2855 (2019)

56. B. Bhattacharya, N. Seriani, U. Sarkar, "Raman and IR signature of pristine and BN-doped gamma-graphyne", Carbon 141, 652 (2018)

55. M. Corva, A. Ferrari, M. Rinaldi, Z. Feng, M. Roiaz, C. Rameshan, G. Rupprechter, G. Pastore, G. Comelli, N. Seriani, E. Vesselli, "Vibrational fingerprint of localized spin excitons in a 2D metalorganic crystal", Nature Communications 9, 4703 (2018)

54. M. Corva, F. Mohamed, E. Tomsic, Z. Feng, T. Skala, G. Comelli, N. Seriani, M. Peressi, E. Vesselli, "Substrate- to laterally-driven self-assembly steered by Cu nanoclusters: the case of FePcs on an ultrathin alumina film", ACS Nano 12, 10755 (2018)

53. K. Ulman, E. Poli, N. Seriani, S. Piccinin, R. Gebauer, "Understanding the electrochemical double layer at the hematite/water interface: A first principles molecular dynamics study", Journal of Chemical Physics 150, 041707 (2019)

52. L. Tchibota Poaty, K. Ulman, N. Seriani, B. M'Passi Mabiala, R. Gebauer, "Characterization of peroxo reaction intermediates in the water oxidation process on hematite surfaces", Journal of Molecular Modeling 24, 284 (2018)

51. V. Meng'wa, N. Makau, G. Amolo, S. Scandolo, N. Seriani; "A Density Functional Theory Study of Water Photo-oxidation at Copper Oxide Nanostructures on the Anatase (101) Surface", The Journal of Physical Chemistry C 122, 16765 (2018)

50. S. A. H. Abass, N. Seriani, "Structural and electronic properties of $Na_2Ti_3O_7$ and $H_2Ti_3O_7$", Physica Status Solidi B 1700612 (2018)

49. I. Ahamed, K. Ulman, N. Seriani, R. Gebauer, A. Kashyap, "Magnetoelectric epsilon-Fe_2O_3: DFT study of a potential candidate for electrode material in photoelectrochemical cells", Journal of Chemical Physics 148, 214707 (2018)

48. N. Seriani, "Ab initio simulations of water splitting on hematite", Journal of Physics: Condensed Matter 29, 463002 (2017)

47. V. Meng'wa, N. Makau, G. Amolo, S. Scandolo, N. Seriani, "Ab initio simulations of copper oxide nanowires and clusers on TiO_2 (101) anatase surface", The Journal of Physical Chemistry C 121, 20359 (2017)

46. N. Ansari, K. Ulman, M. Farnesi Camellone, N. Seriani, R. Gebauer, S. Piccinin, "Hole localization in Fe_2O_3 from density functional theory and wavefunction-based methods", Physical Review Materials 1, 035404 (2017)

45. J. Songkhao, R. Banerjee, S. Debnath, S. Narasimhan, N. Wannaprom, P. Vanalabhpatana, N. Seriani, R. Gebauer, P. Thamyongkit, "Structure-property Relationship of Pi-Extended Boron-dipyrromethene Derivatives towards Optoelectronic Applications", Dyes and Pigments 142, 558 (2017)

44. S. S. Ataei, M. R. Mohammadizadeh, N. Seriani, "Excitonic effects in the optical properties of hydrogenated anatase TiO_2", Physical Review B 95, 155205 (2017)

43. K. Ulman, M.-T. Nguyen, N. Seriani, S. Piccinin, R. Gebauer, "A unified picture of water oxidation on bare and gallium-covered hematite from density functional theory", ACS Catalysis 7, 1793 (2017)

42. N. Seriani, C. Pinilla, S. Scandolo, "Titania-silica mixed oxides investigated with density functional theory and molecular dynamics simulations", Physica Status Solidi B, 1-7 (2016)

41. B. Bhattacharya, U. Sarkar, N. Seriani, "Electronic Properties of Homo and Hetero Bilayer Graphyne: The Idea of a Nanocapacitor", The Journal of Physical Chemistry C 120, 26579 (2016)

40. C. Pinilla, M. Acuna-Rojas, N. Seriani, S. Scandolo, "An atomistic model of $MgSiO_3$ perovskite and post-perovskite phases", Computational Materials Science 126, 351 (2016)

39. E. Araujo-Lopez, L. Alcala Varilla, N. Seriani, J. A. Montoya, "TiO_2 anatase's bulk and (001) surface, structural and electronic properties: A DFT study on the importance of Hubbard and van der Waals contributions", Surface Science 653, 187 (2016)

38. S. S. Ataei, M. R. Mohammadizadeh, N. Seriani, "Ab-initio simulation of the effects of hydrogen concentration on anatase TiO_2", The Journal of Physical Chemistry C 120, 8421 (2016)

37. K. Ulman, M.-T. Nguyen, N. Seriani, R. Gebauer, "Passivation of surface states of alpha-Fe_2O_3 (0001) surface by deposition of Ga_2O_3 overlayers : A Density Functional Theory study", Journal of Chemical Physics 144, 094701 (2016)

36. U. Sarkar, B. Bhattacharya, N. Seriani, "First principle study of sodium decorated graphyne", Chemical Physics 461, 74 (2015)

35. B. H. Cogollo-Olivo, N. Seriani, J. A. Montoya, "Unbiased structural search of small copper clusters within DFT", Chemical Physics 461, 20 (2015)

34. E. Uzunova, N. Seriani, H. Mikosch, "CO_2 conversion to methanol on Cu(I) oxide nanolayers and clusters: an electronic structure insight into the reaction mechanisms", Physical Chemistry Chemical Physics 17, 11088 (2015)

33. N. Seriani, C. Pinilla, Y. Crespo, "Presence of gap states at Cu/TiO_2 anatase surfaces: consequences for the photocatalytic activity", Journal of Physical Chemistry C 119, 6696 (2015)

32. M.-T. Nguyen, N. Seriani, R. Gebauer, "Nitrogen electrochemically reduced to ammonia with hematite: density-functional insights", Physical Chemistry Chemical Physics 17, 14317 (2015)

31. M.-T. Nguyen, S. Piccinin, N. Seriani, R. Gebauer, "Photo-oxidation of water on defective hematite(0001)", ACS Catalysis 5, 715 (2015)

30. S. Mandal, A. Andreanov, Y. Crespo, N. Seriani, "Incommensurate, helical spin ground states on the Hollandite lattice", Physical Review B 90, 104420 (2014)

29. A. Dianat, N. Seriani, L. Colombi Ciacchi, M. Bobeth, G. Cuniberti, "DFT study of reaction processes of methane combustion on PdO(100)", Chemical Physics 443, 53 (2014)

28. Y. Crespo, N. Seriani, "Lithium peroxide precursor on the alpha-MnO_2(100) surface", Journal of Materials Chemistry A 2, 16538 (2014)

27. M.-T. Nguyen, N. Seriani, R. Gebauer, "Defective alpha-Fe_2O_3(0001): an ab-initio study", ChemPhysChem 15, 2930 (2014).

26. M.-T. Nguyen, N. Seriani, S. Piccinin, R. Gebauer, "Photo-driven oxidation of water on alpha-Fe_2O_3 surfaces: an ab initio study", Journal of Chemical Physics 140, 064703 (2014)

25. Y. Crespo, N. Seriani, "Electronic and magnetic properties of alpha-MnO_2 from ab-initio calculations", Physical Review B 88, 144428 (2013)

24. Y. Crespo, A. Andreanov, N. Seriani, "Competing antiferromagnetic and spin-glass phases in a hollandite structure", Physical Review B 88, 014202 (2013)

23. A. Dianat, N. Seriani, M. Bobeth, G. Cuniberti, "Effect of Al-doping on the properties of Li-Mn-Ni-O cathode materials for Li-ion batteries: an ab initio study", Journal of Materials Chemistry A 1, 9273 (2013)

22. M.-T. Nguyen, N. Seriani, R. Gebauer, "Water adsorption and dissociation on alpha-Fe_2O_3(0001): PBE+U calculations", Journal of Chemical Physics 138, 194709 (2013)

21. N. Seriani, "Sodium promoter inducing a phase change in a palladium catalyst", Journal of Physical Chemistry C 116, 22974 (2012)

20. N. Seriani, C. Pinilla, S. Cereda, A. De Vita, S. Scandolo, "Titania-silica interfaces", Journal of Physical Chemistry C 116, 11062 (2012)

19. C. Pinilla, A. Irani, N. Seriani, S. Scandolo, "Ab-initio parametrization of a fully polarizable and dissociable force field for water", Journal of Chemical Physics 136, 114511 (2012)

18. N. Seriani, "A relation between kinetic-energy density and band gap in alkali and alkaline-earth oxides", Journal of Physics: Condensed Matter 22, 255502 (2010)

17. K. Rasim, M. Bobeth, W. Pompe, N. Seriani, "A microkinetic model of ammonia decomposition on a Pt overlayer on Au(111)", Journal of Molecular Catalysis A: Chemical 325, 15 (2010)

16. N. Seriani, F. Mittendorfer, G. Kresse, "Carbon in palladium catalysts: a metastable carbide", Journal of Chemical Physics 132, 024711 (2010)

15. A. Dianat, N. Seriani, L. Colombi Ciacchi, W. Pompe, G. Cuniberti, M. Bobeth, "Dissociative adsorption of methane on surface oxide structures of Pd-Pt alloys", Journal of Physical Chemistry C 113, 21097 (2009)

14. N. Seriani, "Ab-initio thermodynamics of lithium oxides: from bulk phases to nanoparticles", Nanotechnology 20, 445703 (2009)

13. R. Westerström, C. J. Weststrate, J. Gustafson, A. Mikkelsen, J. Schnadt, J. N. Andersen, E. Lundgren, N. Seriani, F. Mittendorfer, G. Kresse, A. Stierle, "Lack of surface oxide layers and facile bulk oxide formation on Pd(110) ", Physical Review B 80, 125431 (2009)

12. N. Seriani, J. Harl, F. Mittendorfer, G. Kresse, "A first-principles study of bulk oxide formation on Pd(100)", Journal of Chemical Physics 131, 054701 (2009); **JCP Editor's choice 2009**

11. M. Kralj, T. Pertram, N. Seriani, C. Becker, A. Krupski, F. Mittendorfer, K. Wandelt, "Pd(110) surface oxide structures investigated by STM and DFT", Surface Science 602, 3706 (2008)

10. A. Dianat, N. Seriani, M. Bobeth, W. Pompe, L. Colombi Ciacchi, " DFT study of the thermodynamic stability of Pd-Pt bulk oxide phases", Journal of Physical Chemistry C 112, 13623 (2008)

9. R. Westerström, C. J. Weststrate, A. Resta, A. Mikkelsen, J. Schnadt, J. N. Andersen, E. Lundgren, M. Schmid, N. Seriani, J. Harl, F. Mittendorfer, G. Kresse, "Stressing Pd atoms: initial oxidation of the Pd(110) surface", Surface Science 602, 2440 (2008)

8. N. Seriani, F. Mittendorfer, "Platinum-group and noble metals under oxidizing conditions", Journal of Physics: Condensed Matter 20, 184023 (2008)

7. A. Dianat, J. Zimmermann, N. Seriani, M. Bobeth, W. Pompe, L. Colombi Ciacchi, "Ab initio study of element segregation and oxygen adsorption on PtPd and CoCr binary alloy surfaces", Surface Science 602, 876 (2008)

6. F. Mittendorfer, N. Seriani, O. Dubay, G. Kresse, "The morphology of mesoscopic Rh and Pd nanoparticles under oxidizing conditions", Physical Review B 76, 233413 (2007)

5. N. Seriani, Z. Jin, W. Pompe, L. Colombi Ciacchi, "A DFT study of platinum oxides: from infinite crystals to nanoscopic particles", Physical Review B 76, 155421 (2007); **Selected for the 5^{th} November, 2007 issue of the Virtual Journal of Nanoscale Science and Technology**

4. R. Westerström, J. Gustafson, A. Resta, A. Mikkelsen, J. N. Andersen, E. Lundgren, N. Seriani, F. Mittendorfer, M. Schmid, J. Klikovits, P. Varga, M. D. Ackermann, J. W. M. Frenken, N. Kasper, A. Stierle, "Oxidation of Pd(553): from ultrahigh vacuum to atmospheric pressure", Physical Review B 76, 155410 (2007)

3. J. Klikovits, E. Napetschnig, M. Schmid, N. Seriani, O. Dubay, G. Kresse, P. Varga, "Surface oxides on Pd(111): STM and density functional calculations", Physical Review B 76, 45405 (2007)

2. P. Kostelník, N. Seriani, G. Kresse, A. Mikkelsen, E. Lundgren, V. Blum, T. Šikola, P. Varga, M. Schmid "The Pd(100)-($\sqrt{5} \times \sqrt{5}$)R27°-O surface structure: a LEED, DFT and STM study", Surface Science 601, 1574-1581 (2007)

1. N. Seriani, W. Pompe, L. Colombi Ciacchi, "Catalytic oxidation activity of Pt_3O_4 surfaces and thin films", Journal of Physical Chemistry B 110, 14860-14869 (2006)

Citations

Hirsch-index (H-index): 29 (from ISI Web of Knowledge)

Talks

- "Theoretical insight into hematite as a photoelectrode for water splitting", 30th September 2024, at the XXII Meeting of the Brazilian Materials Research Society (XXII B-MRS Meeting), in Santos (Brazil); **Invited talk**
- "Ab-initio simulations of materials for energy applications", 26th September 2024, at the "Advanced functional materials for next generation thin film photovoltaics" Conference, in Samarkand (Uzbekistan); **Invited talk**
- "Catalytic production of solar fuels" (in Italian), 21st September 2024, at the Scuola di Introduzione alle Energie Rinnovabili (SIER 2024), in Udine (Italy); **Invited talk**
- "Ab initio simulations for energy applications", 20th September 2024, at PWF Tunisia: Computational Materials Science based on Density-Functional Theory for Renewable Energy and Spintronics PWF Tunisia in Tunisi (Tunisia), virtual talk at a hybrid school; **Invited talk**
- "Computational materials science for functional materials: fundamental science for development", 20th September 2024, at PWF Tunisia: Computational Materials Science based on Density-Functional Theory for Renewable Energy and Spintronics PWF Tunisia in Tunisi (Tunisia), virtual talk at a hybrid school; **Invited talk**
- "Synergy of doping and nanostructuring of oxide photocatalysts", 21st August 2024, at the 32nd International Materials Research Congress 2024 IMRC 2024 in Cancun (Mexico), virtual talk at a hybrid conference; **Invited talk**
- "Understanding materials at the atomic scale through ab-initio simulations", 3rd July 2024, at the 21st International Conference for Laser Optics ICLO 2024 in Saint Petersburg (Russia), virtual talk at a hybrid conference; **Invited talk**
- "Computational materials science for functional materials", 5th June 2024, at the University of Technology and Applied Sciences in Muscat (Oman), virtual
- "Ab-initio simulations of materials for energy applications", 16th April 2024, at the WIEN2k Hands-On Workshop for New and Existing Users in Trieste (Italy)
- "Novel hybrid perovskites from ab-initio simulations", 4th October 2023, at the XXI Meeting of the Brazilian Materials Research Society (XXI B-MRS Meeting) in Maceio (Brazil) **Invited talk**

- "Theory and ab-initio simulations of oxide photocatalysts", 15th September 2023, at the Webinar "New results in nanophysics, bionanoscience, nanophotonics, and solar energy conversion", organised by the Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Magurele-Bucharest (Romania)

- "Ab-initio simulations of materials for energy applications", 2nd September 2023, at the 39th Turkish Physical Society International Physics Congress in Bodrum (Turkey) **Invited talk**

- "Computational materials science for functional materials: fundamental science for development", 8th June 2023, at the PWF Rwanda - School on Computational Materials Science (virtual talk at a school in presence)

- "Catalytic production of solar fuels" (in Italian), 22nd September 2022, at the Scuola di Introduzione alle Energie Rinnovabili, in Udine (Italy) **Invited talk**

- "Clusters in the sun: ab-initio design of cluster-based hybrid perovskites", 14th August 2022, at the Psi-k conference in Lausanne (Switzerland)

- "Insight into the electrochemical interface at a hematite photoelectrode from theory and simulations", 16th August 2022, at the XXX International Materials Research Congress , hybrid conference in Cancun (Mexico) **Invited talk**

- "Theory and ab-initio of oxide photocatalysts simulations", 22nd February 2022, at the International Conference on Solid State Physics (ICSSP'21), hybrid conference in Lahore (Pakistan) **Invited talk**

- "Introduction to Density Functional Theory", 16th February 2022, at the Second Adriatic Conference on Strongly Correlated Systems (and beyond), on-line

- "Catalytic production of solar fuels" (in Italian), 17th September 2021, at the Scuola di Introduzione alle Energie Rinnovabili, in Udine (Italy) **Invited talk**

- "Characterisation of photoelectrodes through computer simulations", 25th August 2021, at the International Conference on Thin films and Nanotechnology - Knowledge, Leadership and Commercialization (ICTN-KLN, India), on-line **Invited talk**

- "Ab-initio simulations of an electrochemical interface", 4th June 2020, at the African School for Fundamental Physics, on-line **Invited talk**

- "Ab-initio simulations of an electrochemical interface", 10th February 2020, at the 35th Workshop on Novel Materials and Superconductors, in Schladming (Austria) **Invited talk**

- "Computational catalysis", 23rd January 2020, at the African School of Catalysis, in Kigali (Rwanda) (via Skype) **Invited talk**

- "Ab-initio simulations of water oxidation at a hematite surface", 12th December 2019, at the African Materials Research Society conference, in Arusha (Tanzania) **Invited talk**

- "Catalytic production of solar fuels" (in Italian), 7th September 2019, at the Scuola di Introduzione alle Energie Rinnovabili, in Udine (Italy) **Invited talk**

- "Characterization of photoelectrochemical processes for energy conversion through computer simulation", 13th June 2019, at the NanoInnovation2019, in Rome (Italy) **Invited talk**

- "Characterization of photoelectrochemical processes for energy conversion through computer simulations", 31st May 2019, at the ICTP Caribbean School on Materials for Clean Energy, in Cartagena de Indias (Colombia)

- "Understanding water splitting on hematite through computer simulations", 17^{th} October 2018, at the Ethiopian Regional Workshop on Solar Energy and Energy Storage Technologies: Materials, System Design, and Applications in Addis Ababa (Ethiopia).

- "Photoelectrochemistry of water splitting from first principles", 18^{th} September 2018, at the International Workshop on Advances in Nanomaterials in Bucharest (Romania).

- "Ab-initio simulations of photocatalysts for hydrogen production", 14^{th} December 2017, at the 9^{th} International Conference of the African Materials Research Society (AMRS2017) in Gaborone (Botswana).

- "Multifaceted behaviour of hydrogen in titania", 4^{th} October 2017, at the FisMat 2017, the Italian National Conference on Condensed Matter Physics, in Trieste (Italy).

- "Ab-initio simulations of transition metal oxides for energy conversion and storage", 12^{th} September 2017, at the XVI Brazil Materials Research Society Meeting in Gramado (Brazil). **Invited talk**

- "Splitting water on iron oxide", 15^{th} January 2017, at the Khartoum Workshop on Advances in Materials Science (KWAMS'17) in Khartoum (Sudan).

- "Understanding materials at the atomic scale", 5^{th} October 2016, Alumnorum Colloquium at the Department of Physics of the University of Trieste (Italy).

- "Ab-initio simulations of water splitting on hematite", 30^{th} September 2016, at the CECAM Workshop "Interface processes in photochemical water splitting: Theory meets experiment" in Lausanne (Switzerland). **Invited talk**

- "Hematite as a photocatalyst", 26^{th} July 2016, at the Workshop on Radiation-Matter Interactions and Catalysis in Cartagena (Colombia). **Invited talk**

- "Heterogeneous catalysis on platinum and palladium", 26^{th} July 2016, at the Workshop on Radiation-Matter Interactions and Catalysis in Cartagena (Colombia). **Invited talk**

- "Ab-initio investigation of hematite photocatalysts for the production of solar fuels", 22^{nd} July 2016, at the School on Computational Materials Science for Industrial Applications in Barranquilla (Colombia). **Invited talk**

- "Fundamental materials research for applications in heterogeneous catalysis", 22^{nd} July 2016, at the School on Computational Materials Science for Industrial Applications in Barranquilla (Colombia). **Invited talk**

- "Designing battery cathode materials by first-principles simulations: the case of aluminium doping of the Li-Mn-Ni-O system", 3^{rd} May 2016, at the "E-MRS Conference" in Lille (France).

- "Ab-initio simulations of water splitting on hematite", 8^{th} March 2016, at the "DPG Conference" in Regensburg (Germany).

- "Structure of hematite(0001) and water splitting mechanism from ab-initio simulations", 19^{th} October 2015, at the European Conference on Surface Crystallography and Dynamics in Trieste (Italy). **Invited talk**

- "Ab-initio simulations of water splitting on hematite", 2^{nd} September 2015, at the workshop "Advances in Nanophysics and Nanophotonics" in Bucharest (Romania).

- "Ab-initio simulations of functional materials for energy applications", 3^{rd} June 2015, Physics Colloquium via Skype at the African University of Science and Technology (AUST) in Abuja (Nigeria).

- "An introduction to density functional theory", 26^{th} May 2015, at the ICTP Summer School "Modern Trends in Theoretical Condensed Matter Physics: From Low-Dimensional Nanoscale Systems to Advanced Materials for Photovoltaic" in Khiva (Uzbekistan).

- "Fundamental materials research for solar-energy applications", 25^{th} May 2015, at the ICTP Summer School "Modern Trends in Theoretical Condensed Matter Physics: From Low-Dimensional Nanoscale Systems to Advanced Materials for Photovoltaic" in Khiva (Uzbekistan).

- "Formation of lithium peroxide in lithium-air batteries: an ab-initio investigation", 9^{th} February 2015, at the Khartoum Workshop on Advances in Materials Science (KWAMS'15) in Khartoum (Sudan).

- "Ab-initio simulations of hematite as a photocatalyst", 7^{th} February 2015, at the Khartoum Workshop on Advances in Materials Science (KWAMS'15) in Khartoum (Sudan).
- "An ab-initio investigation of the effects of copper on titania photocatalysts", 25^{th} September 2014, at the Materials Science and Engineering conference in Darmstadt (Germany).
- "Titania as a photocatalyst: the effect of copper", 1^{st} September 2014, at the Advanced workshop on solar energy conversion and nanophysics in Bucharest (Romania).
- "Basic materials research for renewable-energy applications", 19^{th} August 2014, at the ASEAN Conference on Science and Technology 2014 in Bogor (Indonesia). **Invited keynote talk**
- "First-principles simulations of platinum and palladium catalysts under oxygen-rich conditions", 3^{rd} July 2014, at the 14^{th} International Balkan Workshop on Applied Physics in Constanta (Romania). **Invited talk**
- "Quantum-ESPRESSO, a software for the study of extended systems - Application to the study of materials for solar energy harvesting", 24^{th} June 2014, at the Institute of General and Inorganic Chemistry of the Bulgarian Academy of Sciences in Sofia (Bulgaria).
- "Ab-initio simulations of copper-modified titania photocatalysts", 31^{st} March 2014, at the DPG Conference in Dresden (Germany).
- "Ab-initio simulations of platinum and palladium catalysts under oxygen-rich conditions", 7^{th} March 2014, at the University of the North in Barranquilla (Colombia). **Invited talk**
- "Ab-initio simulations of platinum and palladium catalysts under oxygen-rich conditions", 7^{th} March 2014, at the University of Cartagena in Cartagena (Colombia). **Invited talk**
- "Titania as a photocatalyst: the effect of copper", 2^{nd} December 2013, at the International Conference on Solid State Physics 2013 in Lahore (Pakistan). **Invited talk**
- "Ab-initio simulations of photocatalytic systems", 5^{th} November 2013, at the Regional Workshop on Materials Science for Solar Energy Conversion in Cape Town (South Africa).
- "Ab-initio simulations of copper-modified titania photocatalysts", 23^{rd} September 2013, at the workshop 'New trends in nanophysics and solar energy conversion' in Bucharest (Romania).

- "First-principles simulations of a copper-modified titania photocatalyst", 9^{th} September 2013, at the EUROMAT 2013 conference in Sevilla (Spain).
- "Ab-initio simulations of materials for lithium-air batteries", 23^{rd} July 2013, at the CECAM Summer School on Atomistic Simulation Techniques at SISSA in Trieste (Italy).
- "Ab-initio simulations of platinum-group metal catalysts under oxygen-rich conditions", 6^{th} July 2013, at the 13^{th} International Balkan Workshop on Applied Physics in Constanta (Romania). **Invited talk**
- "Simulations of materials for lithium-air batteries", 27^{th} June 2013, at the Third LinkSCEEM General User Meeting in Alexandria (Egypt). **Invited talk**
- "Ab-initio simulations of copper-modified titania photocatalysts", 22^{nd} March 2013, at the Second International Advanced Materials Science Networking (AMASING) Workshop in Da Nang (Vietnam). **Invited talk**
- "Computational materials science for energy applications", 24^{th} January 2013, at the 1^{st} Khartoum Workshop on Advances in Materials Science (KWAMS'13) in Khartoum (Sudan).
- "Simulation of Li-air batteries", 28^{th} November 2012, at the School on Numerical Methods for Materials Science Related to Renewable Energy Applications in Trieste (Italy).
- "Atomistic simulations of oxides and water: from first principles to classical polarizable potentials", 14^{th} November 2012, at the Atomistic Modelling for Industrial Product Development workshop in Bremen (Germany).
- "An ab-initio investigation of the reversible formation of lithium oxides in lithium-air batteries", 26^{th} September 2012, at the Materials Science and Engineering (MSE 2012) conference in Darmstadt (Germany).
- "Investigation of cathode materials for lithium-air batteries by ab-initio computer simulations", 21^{st} August 2012, at the International Conference on Materials Science in Ulaanbaatar (Mongolia).
- "Ab-initio simulations of cathode materials for lithium-air batteries", 8^{th} June 2012, at the Workshop AMASING (Alumni Materials Science Networking) - Applications of nanotechnology in modern energy concepts in Dresden (Germany). **Invited talk**
- "Computational materials science for energy applications", 22^{nd} May 2012, at the Advanced workshop on solar energy conversion in Bucharest (Romania).

- "Atomistic simulations of surface oxides and oxide surfaces from first principles", 16^{th} June 2011, at the Quantitative Micro-Nano 2 (QMN-2) Workshop in Sun Valley (Idaho, USA). **Invited talk**
- "Lithium oxide nanoparticles in lithium-air batteries: an ab-initio study", 17^{th} March 2011, at the DPG Conference in Dresden (Germany).
- "Ab-initio parameterisation of inter-atomic force fields for the description of solid-solid and liquid-solid interfaces ", 14^{th} March 2011, at the DPG Conference in Dresden (Germany).
- "Silica-modified titania photocatalysts: a computational investigation", 14^{th} March 2011, at the DPG Conference in Dresden (Germany).
- "Energy conversion and storage with nanomaterials: atomistic simulations", 3^{rd} March 2011, Special Seminar at the ICTP in Trieste (Italy).
- "Polarizable potentials for classical molecular dynamics", 11^{th} November 2010, at the Mini Workshop on Atomistic Modelling of the FP7 project ADGLASS in Bremen (Germany).
- "Development of an inter-atomic force field for the water/a-SiO_2 and a-SiO_2/TiO_2 interfaces", 10^{th} November 2010, at the Mini Workshop on Atomistic Modelling of the FP7 project ADGLASS in Bremen (Germany).
- "Ab-initio investigations of platinum oxides", 16^{th} March 2010, at TASC-INFM National Laboratory in Trieste (Italy).
- "Carbon in palladium catalysts", 26^{th} March 2009, at DPG Conference in Dresden (Germany).
- "Palladium in selective hydrogenation catalysis", 3^{rd} November 2008, at IUVSTA Workshop in Schlaining (Austria).
- "Simulation of Pd oxide films on Pd(100) by density functional theory and genetic algorithms", 30^{th} July 2008 at ECOSS-25 Conference in Liverpool (United Kingdom).
- "Oxidation of Palladium Surfaces and Nanoparticles", 28^{th} February 2008 at DPG Conference, Berlin (Germany).
- "Oxidation of Transition Metal Surfaces and Nanoparticles", 13^{th} September 2007 at EUROMAT conference, Nuremberg (Germany).
- "Pt and Pd under oxidizing conditions: a first-principles investigation of surfaces and nanostructures", 26^{th} February 2007 at IfWW, TU Dresden (Germany).
- "Morphology of transition metal clusters under high oxygen pressure: a first-principles investigation", 28^{th} September 2006 at NanO2 Workshop, Kloster Irsee (Germany).

- "Ab-initio simulations of materials properties", 27^{th} February 2006 at TUHH, Hamburg (Germany).
- "Ab-initio thermodynamics and adsorption properties of platinum oxides", 4^{th} October 2005 at ELETTRA Laboratory in Trieste (Italy).
- "Ab-initio thermodynamics of platinum oxides", 19^{th} July 2004 at IMWF Stuttgart (Germany).

Teaching and Mentoring

- Supervisor of one Ph.D. student at the University of Trieste. Paola A. Delcompare-Rodriguez graduated in 2022 with a thesis entitled "A theoretical investigation of ultrathin space charge layers in hematite photoelectrodes" and joined CNR-IOM as a postdoc.
- Co-supervisor of four Ph.D. students in the framework of the Sandwich Training Education Programme (STEP). Mohamed El-Kinawy (Ain Shams University, Egypt) is expected to finish his PhD in 2024. Samaneh Ataei (University of Tehran, Iran) graduated in 2017 and joined the University of Modena and Reggio Emilia as postdoc. Victor Meng'wa (University of Eldoret, Kenya) graduated in 2018 and is now lecturer at the Alupe University College, Sara Abass (University of Khartoum, Sudan) graduated in 2019 and is now lecturer at the University of Khartoum.
- Co-supervisor of two Ph.D. students at EAIFR: Sunday Ogenyi and Wala El-Sayed.
- Supervisor of three Master theses. Two at the University of Trieste: that of Ifeanyi John Onuorah (2015) and that of Gemechis Dereje Degaga (2013). Ifeanyi John Onuorah defended a thesis entitled "Ab-initio simulations of sodium superoxide" with a final grade of 104/110. He started his PhD studies at the University of Parma in autumn 2015. Gemechis Dereje Degaga defended a thesis entitled "Ab-initio study of electronic structure and structural stability of Cu doped polymorphs of titania" with a final grade of 100/110. He has started his PhD studies at the Michigan Technological University (USA) in autumn 2013. One Master thesis at the African University of Science and Technology, that of Sunday Joseph Ogenyi (2016), with a thesis entitled "Optical properties of metal clusters from first principles calculations".
- Co-supervisor of three Master theses at the University of Trieste: that of Alex Pividori (2019, with Erik Vesselli), that of Matteo Rinaldi (2017, with Erik Vesselli), that of Alberto Ferrari (2016, with Erik Vesselli) and that of Sadhana Chalise (2013, with Sandro Scandolo). Alex Pividori defended a thesis entitled "Interaction of molecular oxygen with cobalt tetrapyridylporphyrins: an ab initio investigation", with a final grade of 100/110. Matteo Rinaldi defended a thesis entitled "Adsorption of CO and CO_2 on iron phthalocyanines: an ab initio investigation of structural, electronic, and

vibrational properties" with a final grade of "110/110 e lode", and started a PhD at the Ruhr University Bochum in January 2018. Alberto Ferrari defended a thesis entitled "Ab-initio investigation of reactivity, electronic and vibrational properties of iron phthalocyanines" with a final grade of "110/110 e lode", and started a PhD at the Ruhr University Bochum in autumn 2016. Sadhana Chalise defended a thesis entitled "Vibrational properties of TiO_2 nanoparticles from atomistic simulations" with a final grade of 100/110, and started a PhD at the University of Massachusetts Amherst in autumn 2013.

- Co-supervisor of one Master thesis at EAIFR, Rwanda. Kossi Kety defended his M.Sc. thesis entitled "Machine Learning Interatomic Potential for a Transition Metal Dichalcogenide MoS_2" in April 2022, co-supervised with Samare Rostami (ICTP). Kossi Kety started a PhD at the Universite' Gustave Eiffel in Paris, France, in 2022.

- Supervisor of seven ICTP Postgraduate Diploma theses, those of Nasiru Rahamatu (2024), Areeda Ayoub (2023), Omolara Bakare (2022), Amar Thakuri (2020), Mariano Cornelio Cap Lopez (2020), Thi Hanh Bui (2015) and of Tran Nguyen Dung (2013). Nasiru Rahamatu defended a thesis with the title "Shape recognition of nanostructures", and started her MSc studies at the University of Pavia in autumn 2024. Areeda Ayoub defended a thesis with the title "Structure of charged hematite surfaces", and started her PhD studies at the University of Houston in early 2024. Omolara Bakare defended a thesis with the title "An analysis of molecular dynamics data on radiation damage in tungsten" and started her PhD studies at VirginiaTech in 2022. Amar Thakuri defended a review thesis with the title "Bulk properties of hybrid perovskite for photovoltaic application". Amar Thakuri started his PhD studies at the University of Houston in 2021. Mariano Cornelio Cap Lopez defended a review thesis with the title "Atomic scale properties of electrochemical interfaces: A literature review". Thi Hanh Bui defended a thesis with the title "Ab-initio Investigation of Tetrachloroaluminate Intercalation in a Graphite Cathode" and started her PhD studies at the University of Hamburg in autumn 2015. Tran Nguyen Dung defended a thesis with the title "Ab-initio investigation of structure and electronic properties of sodium superoxide" and started his PhD studies at SISSA (Italy) in autumn 2013.

- Co-supervisor of eleven ICTP Postgraduate Diploma theses: that of Jaurel Kagho Zanguim (2023, with Martina Stella), that of Rosine Intungane (2023, with Abishek Kumar Adak), that of Huma Nawaz (2022, with Samare Rostami), that of Eduard Araujo Lopez (2018, with E. Poli), that of Erick Odoyo Buko (2015, with A. Hassanali), those of Mirriam Chepkoech and of Felana Noeliarinala Andriambelaza (both 2014, with Y. Crespo), that of Elvira Prisca Mbekwe Pafong (2012, with R. Gebauer); those of Osiris Hermes Ngoma (2012), Eyob Kebede (2011) and Keshav Shrestha (2010), with S. Scandolo. Jaurel Kagho Zanguim defended a thesis with the title "Atomic structure and properties of amorphous molybdenum disulfide (MoS2)" and

will start his PhD studies at the University of Padova (Italy) in autumn 2023. Rosine Intungane defended a thesis with the title "TiO2/water interfaces from Density Functional Tight Binding simulations". Huma Nawaz defended a thesis with the title "Amorphous MoS2 from machine learning interatomic potentials simulation" and started her PhD studies at the University of Houston (USA) in autumn 2022. Eduard Araujo Lopez defended a thesis with the title "Dielectric behavior of doped hematite from first principles" and started his PhD studies at the Karlsruhe Institute of Technology (Germany) in autumn 2018. Erick Odoyo Buko defended a thesis with the title "Understanding the Molecular Origins of Many-Body Effects in Liquid Water with Density Functional Theory" and started his PhD studies at the University of Houston (USA) in autumn 2015. Mirriam Chepkoech defended a thesis with the title "Ab initio thermodynamics of oxygen adsorption and vacancies at the surfaces of α-MnO_2", and started her PhD studies at the University of Witswatersrand (South Africa) in autumn 2015. Felana Noeliarinala Andriambelaza defended a thesis with the title "Spin glass transition on α-MnO_2: a Monte Carlo study", and started her PhD studies at the University of Pretoria (South Africa) in autumn 2015. Elvira Prisca Mbekwe Pafong defended a thesis with the title "Density-functional and post density-functional simulations of small iron clusters" and started her PhD studies at the University of Stuttgart (Germany) in autumn 2012. Osiris Hermes Ngoma defended a thesis with the title "Mixed carbonate-silicate crystals at high pressure" and joined Halliburton SAS Congo in autumn 2012. Eyob Kebede defended a thesis with the title "Ab-initio study of metal hydrides at high pressure" and started his PhD studies at SISSA (Italy) in autumn 2011. Keshav Shrestha defended a thesis with the title "Atomistic Simulation of TiO_2 Nanostructures" and started his PhD studies at the University of Houston (USA) in autumn 2010.

- Lecturer on Quantum Mechanics and Density Functional Theory at the First School on Atomistic Simulations of Biomolecules and Materials Science, 3^{rd}-23^{rd} September 2018 in Arusha (Tanzania).

- Lecturer on Density Functional Theory at the School on Theory and Implementation of Electronic Structure Methods, 27^{th}-31^{st} August 2018 in Dschang (Cameroon).

- Held the course "Approximation and interpolation of simple and complex functions" at the joint ICTP-SISSA Master in High Performance Computing (April 2015, April 2016, April 2017, April 2018, April 2019, April 2020, April 2021, April 2022, April 2023, April 2024, and October 2024).

- Visiting assistant professor at the African University of Science and Technology in Abuja (Nigeria), in April 2014 and March 2017. Taught the course "Advanced Quantum Mechanics" to physics Master's students.

- Held the course "Selected Topics in Condensed Matter Physics" for the ICTP Postgraduate Diploma in Condensed Matter Physics (summer semesters 2011-2024; winter semesters 2012/2013-2024/2025).

- Lectures and hands-on sessions about basics of density functional theory during the Third LinkSCEEM General User Meeting, held at the Bibliotheca Alexandrina in Alexandria (Egypt), 25^{th}-27^{th} June 2013.

- Lectures and hands-on sessions about basics of density functional theory during the 1^{st} Khartoum Workshop on Advances in Materials Science (KWAMS'13), held at the University of Khartoum (Sudan), 19^{th}-26^{th} January 2013.

- Hands-on session about basics of density functional theory during the School on Numerical Methods for Materials Science Related to Renewable Energy Applications, held at ICTP, Trieste (Italy), 26^{th}-30^{th} November 2012.

- 3 lectures concerning exercises of the couse of statistical mechanics for the Diploma students at The Abdus Salam ICTP in Trieste (December 2009).

- 2 lectures concerning first-principles simulation techniques within the course "Computer modelling" for students of materials science in Dresden (academic years 2003/2004 and 2004/2005).

Computing
UNIX, Macintosh, Windows; LaTeX, Office, pico, emacs and vi; FORTRAN programming language; basics of the Message Passing Interface (MPI) for parallel computing; rasmol, xmgrace, xfig, and gimp for graphics.

Languages
Italian (mother tongue), excellent German and English

Graduate Record Examination scores (www.gre.org) (2001)
General: Analytical: 770 (better than 97% of participants); Quantitative: 800 (98%); Linguistic (English): 510 (63%); Physics: 970 (95%)

Memberships and awards
Member of the American Chemical Society (since July 2009).
Italian habilitation for associate professor in theory of condensed matter physics (02/B2) and in theoretical chemistry (03/A2), from 10^{th} April 2017.
Idoneità CNR (qualification as scientist by the Italian Research Council), June 2009.

Various responsibilities and qualifications

- Chair of the executive committee of the African School on Electronic Structure Methods and Applications, 2018-to date.

- Co-organizer of the '7th African School on Electronic Structure Methods and Applications - ASESMA 2023', 12^{th} June - 23^{rd} June 2023, in Kigali (Rwanda).

- Co-organizer of the '21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods', 11^{th} January - 13^{th} January 2023, in hybrid form in Trieste (Italy).

- Co-organizer of the 'Workshop on Electrochemical Energy Storage: Theory, Experiments, and Applications', 5^{th} May - 26^{th} May 2022, on-line.

- Co-organizer of the 'Ab-initio Many-Body Methods and Simulations with the Yambo Code', 4^{th} April - 8^{th} April 2022, in hybrid form in Trieste (Italy).

- Co-organizer of the '6^{th} African School on Electronic Structure Methods and Applications (ASESMA-2020)', 31^{st} May - 11^{th} June 2021, on-line.

- Co-organizer of the 'Workshop on Physics and Chemistry of Solid/Liquid Interfaces for Energy Conversion and Storage', 24^{th} May - 28^{th} May 2021, on-line.

- Co-organizer of the '20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods', 23^{rd} February - 25^{th} February 2021, on-line.

- Co-organizer of the 'On-line Workshop on Excited Charge Dynamics in Semiconductors', 28^{th} September - 30^{th} September 2020.

- Co-organizer of the 'ICTP Caribbean School on Materials for Clean Energy', 30^{th} May - 5^{th} June 2019 in Cartagena (Colombia).

- Co-organizer of the '5^{th} African School on Electronic Structure Methods and Applications (ASESMA-2018)', 22^{nd} October - 2^{nd} November 2018 in Addis Ababa (Ethiopia).

- Co-organizer of the 'Ethiopian Regional Workshop on Solar Energy and Energy Storage Technologies: Materials, System Design, and Applications', 15^{th}-19^{th} October 2018 in Addis Ababa (Ethiopia).

- Scientific co-director of the International Workshop on Advances in Nanomaterials, 17^{th}-19^{th} September 2018 in Bucharest (Romania).

- Member of the local organizing committee of FisMat 2017, the Italian National Conference on Condensed Matter Physics in Trieste, 1^{st}-5^{th} October 2017.

- Co-organizer of the 'Workshop on Spectroscopy and Dynamics of Photoinduced Electronic Excitations' in Trieste (Italy), 8^{th}-12^{th} May 2017.

- Co-organizer of the 'College on Multiscale Computational Modeling of Materials for Energy Applications' in Trieste (Italy), 4^{th}-15^{th} July 2016.

- Co-organizer of the 'School in Computational Condensed Matter Physics: From Atomistic Simulations to Universal Model Hamiltonians' in Trieste (Italy), 7^{th}-25^{th} September 2015.
- Scientific co-director of the workshop 'Advances in nanophysics and nanophotonics' in Bucharest (Romania), 31^{st} August-2^{nd} September 2015.
- Co-organizer of the 'Workshop on materials science for energy storage' in Trieste (Italy), 11^{th}-15^{th} May 2015.
- Scientific co-director of the 'Khartoum Workshop on Advances in Materials Science 2015, KWAMS15' in Khartoum (Sudan), 1^{st}-11^{th} February 2015.
- Scientific co-director of the 'Advanced workshop on solar energy conversion and nanophysics' in Bucharest (Romania), 1^{st}-3^{rd} September 2014.
- Co-organizer of the 'Workshop on materials challenges in devices for fuel solar production and employment' in Trieste (Italy), 19^{th}-23^{rd} May 2014.
- Co-organizer of the 'Regional Workshop on Materials Science for Solar Energy Conversion' in Cape Town (South Africa), 4^{th}-8^{th} November 2013.
- Scientific co-director of the workshop 'New trends in nanophysics and solar energy conversion' in Bucharest (Romania), 23^{rd}-25^{th} September 2013.
- Co-organizer of the School on Numerical Methods for Materials Science Related to Renewable Energy Applications, held at ICTP, Trieste (Italy), 26^{th}-30^{th} November 2012.
- Panelist for the 2012 call for research proposals of the Romanian National Research Council (CNCS) in the field of materials science.
- Associate Editor of the African Review of Physics (since spring 2016).
- Referee for Physical Review Letters, the Journal of the American Chemical Society, Energy & Environmental Science, Physical Chemistry Chemical Physics, Langmuir, The Journal of Physical Chemistry, Physical Review B, Journal of Materials Chemistry, Solid State Communications, Surface Science, Applied Surface Science, Physica B, Philosophical Magazine and Journal of Nanoparticle Research.
- Speaker at the course on energy for journalists organized by the FVG Association of Journalists (6^{th} June 2022)
- Speaker at the Italian Quantum Weeks (14^{th} April 2022)
- TV guest at Trieste in Diretta on Telequattro (15^{th} March 2022):

  https://telequattro.medianordest.it/17722/trieste-in-diretta-15-03-2022-1730/

- Radio guest at Laser on Radio Rai 1 (12^{th} April 2022):

  http://www.sedefvg.rai.it/dl/portali/site/articolo/ContentItem-7270551c-a2e6-40d3-8f20-e6c93d865a25.html

- Speaker for the Flash Forward project, series of teleseminars on popular science for high-school students in the region Friuli-Venezia Giulia (10^{th} April 2013 and 26^{th} May 2014).

- Speaker at the Researchers' Night, an outreach event for the general public (27^{th} September 2013).

- Representative of the Postdocs Fellows of the Condensed Matter and Statistical Physics Section (2010-2011).

- Board member of the cycling club S.C. Cottur (since 2010).

- Participation at an intercultural training seminar at the TU Dresden (13^{th} June 2009).

- Responsible of the Sprachduo-Wien project, language tandem program with 300 participants per semester (2006-2012).

- System administrator and webmaster at the Chair of materials science and nanotechnology January 2005 - March 2006.

- Organizer of the series of internal seminars of the Chair of materials science and nanotechnology September 2005 - March 2006.

- Founder of AEGEE-Dresden, the local section of the European Students' Forum (October 2003).

- Student representative in the council for the physics degree course in Trieste (academic year 1999/2000).

- Childrens' trainer for the cycling club S.C.V. Cottur (1998-2000).