Curriculum Vitae Marcella Iannuzzi

PERSONAL INFORMATION

Born February 26th, 1973 in Milano, Italy
Nationality: Italy/Switzerland
Languages: Italian (mother tongue), English, German, French
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CURRENT POSITION

Professor and Group Leader for *Computational Materials Science*
University of Zurich, Department of Chemistry

EDUCATION

1997–2001	Ph.D. in Materials Science – University of Milano-Bicocca, Milano, Italy
1991–1997	Undergraduate Physics courses at the University of Milano, Italy (Italian "Laurea", final grant 110/110, cum Laude)

PROFESSIONAL AND ACADEMIC EXPERIENCE

Since 2023	Professor, group of "Computational Materials Science" at the Department of Chemistry, University of Zurich, Switzerland
2019–2022	Privatdozentin, group leader in "Computational Materials Science" at the Department of Chemistry, University of Zurich, Switzerland
2017–2018	Privatdozentin, research associate in the Department of Chemistry, University of Zurich, Switzerland
12/2016	Habilitation (*Venia Legendi*) in computational Materials Science, Received from the Faculty of Science of the University of Zurich, Switzerland *Dissertation*: *Hexagonal Boron Nitride and Graphene Supported on Transition Metals: Density Functional Theory for Large Scale Simulations*
2012–2016	Research associate in the group of Prof J. Hutter, University of Zurich, Switzerland
2009–2011	Post-doc fellowship in the group of Prof J. Hutter, University of Zurich, Switzerland
2008	Leader of the activities of Work Package: *Multiscale modelling exercise on uranium dioxide: transport and thermo-mechanical properties*, for the EU-FP7 project F-Bridge.
2007–2008	Researcher in the group of Core and Fuel Behaviours in the department for Nuclear Energy and Safety, at Paul Scherrer Institute, Switzerland.
2005–2006	Post-doc fellowship in the group of Prof Hutter, University of Zurich, Switzerland.
2001–2004	Post-doc fellowship in the group of Prof Parrinello at the ETH Zurich - CSCS, Switzerland
2001	Post-doc fellowship in the group of Prof Parrinello at the Max-Planck Institute of solid state research, Stuttgart, Germany
2000	Consultant for ST-Microelectronics in collaboration with the soft-computing group located in Catania, Italy

FUNDED RESEARCH PROJECTS AS LEADING INVESTIGATOR

2024-2027	Sinergia Project *Making Carbon-Carbon Bond from CO2: from Discovery to Molecular-Level Understanding and Guiding Principles,* (co-PI with C. Coperet, C. Müller, O. Sefonova) **1'977'874 CHF**
2022–2026	SNSF Project *Light Induced Processes and Core Level Spectroscopy from Real-Time Time Dependent Density Functional Theory for Condensed Matter Systems,* **573'759**. **CHF**
2020–2021	UZH-HUB Joint Seed Money Funding: *Light-induced dynamics of 2D hexagonal boron nitride and its hybrid interfaces* **8'000 CHF** (together with C. Cocchi, Humbold University Berlin)

2016–2018 SNSF Project: *Density Embedding Methods for Condensed Phase Systems,* **334'926 CHF** (together with J. Hutter UZH)

2013–2015 KTI research project: *Toward better performing alignment films for the LCD industry: a computationally inspired strategy*, **930'000 CHF** (together with EMPA and ROLIC)

2012–2015 SNSF Project: *Atomistic simulations of molecules at interfaces,* **313'956 CHF** (together with J. Hutter, UZH)

2010–2012 CCMX project: *Development of computational tools for molecular modeling and X-ray spectroscopy, with application to the understanding and design of molecular alignment technology in commercial LCDs,* **413'000 CHF** (together with EMPA and ROLIC)

2008-2009 WorkPackage "Multiscale modelling exercise on uranium dioxide: transport and thermo-mechanical properties", as part of the EU-FP7 project F-Bridge (one postdoc for 2 years at PSI)

SUPERVISION OF JUNIOR RESEARCHERS

Supervised PhD Theses

- Yun Ding, "Investigation of Molecule Adsorption on h-BN Nanomesh: Water and Phthalocyanine", University of Zurich, 2012
- Samuele Giani, "Calculationsof Spectroscopical Properties of Extended Systems", Universityof Zurich, 2014
- Konstanze Hahn, "Computer Simulations of Chemical Reactionson Metal Oxide Surfaces", University of Zurich, 2013

Supervised PhD Theses and in promotion committee

- Dorothea Golze, "Efficient Methods to Reduce the Complexity of the Charge Density Functional Theory for Large Systems", University of Zurich, 2016
- Ralph Koitz, "Functional Two-Dimensional Materials: A Computational Study of Complex Processes at Interfaces", University of Zurich, 2015
- Florian Hodel "Computational Investigations of Biomimetic Co(II)-Based Water Oxidation Catalysts", University of Zurich, 2016
- Yeliz Guerdal, "Theoretical Investigation of H_2 Generation Systems: From Homogenous to Heterogeneous Photo-Catalysis", University of Zurich, 2017
- Jinggang Lan, "Ab initio Simulations of Condensed Aqueous Systems", University of Zurich, 2020
- Michela Pauletti, "Computational Investigations of Liquid Systems: a Journey from Classical to Quantum Methods", University of Zurich, 2021
- Fabian Belleflamme, "Combining Accuracy with Linear-Scaling Efficiency: A Variational Formulation of the Harris Functional as Correction to Subsystem DFT", University of Zurich, 2022
- Fernanda Nunes, "Tackling electronic and nuclear dynamics at different timescales", University of Zurich, 2023

Currently supervised PhD students (in promotion committee): Maria Bilichenko, Nanchen Dongfang, André Nyberg Borrfors, Florian Keller, Nicolas Tavernier, Xinyue Sun

Supervised Master Theses: David Sidler, Thomas Kedzierski, Pauline Bacle (ENS Paris), Corina Keller, Chiara Cignarella (Universitá La Sapienza Roma), Noah Baumann, Charlotte Mueller, Nanchen Donfang, Ginea D'Ercole, Pierre Marmey (ENS-Lyon), Casper Camenisch, Yuncheng Liu

Supervised Postoctoral Researchers: Marie-Lore Bonnet, Sebastiano Caravati, Tiziana Musso, Gabriele Tocci, Giacomo Melani, Yasmine Al-Hamdani, Guillaume Le Breton, Michael R. Coates

TEACHING ACTIVITIES (University of Zurich)

2017–2019 Condensed Matter Electronic Structure Theory, Master course, 3 hours/week, 14 weeks.

Since 2012 Statistical Mechanics and Molecular Simulations, Bachelor course, 6 hours/week, 7 weeks.

Since 2020 Surface and Interface Science, Master course, 3 hours/week, 14 weeks.

INSTITUTIONAL RESPONSIBILITIES

Since 2020 Board member of the Graduate School of Chemical and Molecular Sciences Zurich (CMSZH)
Since 2024 IT manager for the Chemistry Department of the University of Zurich

INDIVIDUAL SCIENTIFIC REVIEWING ACTIVITIES

External PhD Defenses and Thesis Reports:
(1) Alessandro Lunghi, Universitá di Firenze (Prof. F. Totti) **(2)** Guglielmo Fernandez Garcia, Universite de Rennes (Dr. B. Le Guennic); **(3)** Iurii Zhovtobriukh, Stockholm University (Prof. L. Pettersson); **(4)** Matteo Briganti, Universitá di Firenze (Prof. F. Totti); **(5)** Benoît Grosjean, Ecole Normal Superiore Paris (Dr. M. Bocquet); **(6)** Kana Ishisoone, Strasbourg University (Prof. M. Boero); **(7)** Sander Hanslin, NTNU Norwegian Univrsity of Science Technology (Prof. J. Accola), **(7)** Berta Martinez Bachs, Universitat Autònoma de Barcelona, Spain (Prof. Albert Rimola)**.**

Reviewer for Peer-reviewed Journals
2D Materials, ACS Catalysis, Angewandte Chemie, Carbon, Journal of American Chemical Society**,** Journal of Chemical Theory and Computation, Journal of Physical Chemistry C, Physical Review Letters, Nanotechnology, npj Computational Materials, Nature Catalysis, Nature Communications, The Journal of Chemical Physics, Journal Electronic Structure.

Reviewer of research projects for
France–Agence National de la Recherche, The Dutch Research Council, Partnership for Advanced Computing in Europe, Regular Fondecyt National Projects Competition of Chile

MAJOR PRESENT COLLABORATIONS

Since 2015 Prof M. Odelius, Department of Physics, Stockholm University, Sweden,
on *"Core level spectroscopy and electron dynamics in complex condensed matter systems"*
Since 2019 Dr C. Cucinotta, Imperial College London, London, UK,
on *"Development of methodologies to simulate electrochemical devices"*
Since 2021 Prof D. Passerone, EMPA, Dübendorf, Swizerland,
on *"Disentangling non-local vdW interactions at surfaces"*
Since 2022 Prof F. Nattarer, Department of Physics, University of Zurich, Switzerland,
on *"Spin Polarized STM and magnetism at surfaces"*
Since 2022 Prof C. Coperet, Department of Chemistry, ETH Zurich, Switzerland,
on *"Design of catalytic processes for CO2RR"*
Since 2024 Prof. F. Totti, Universitá di Firenze, "*Investigation magnetic systems in hybrid scenarios by ab initio approaches*"
Since 2024 Dr. Luca Artiglia, Prof. J.A. Bokhoven Paul Scherrer Institute, ETH Zurich, "*Characterization of epoxidation processes under reaction conditions*"

PEER REVIEWED SCIENTIFIC PUBLICATIONS

- Zhao, Y.; Dongfang, N.; Huang, C.; Erni, R.; Li, J.; Zhao, H.; Pan, L.; Iannuzzi, M.; Patzke, G. R. Operando Monitoring of the Functional Role of Tetrahedral Cobalt Centers for the Oxygen Evolution Reaction. *Nat. Commun.*, *16* (1), 580 (2025).
- Patzke, G. R.; Keller, F.; Iannuzzi, M.; Reith, L.; Marshall, K. P.; Beek, W. van; Triana, C. A. Structure-Selection Dynamics of Cobalt Nanoparticles from Solution Synthesis and Their Impact on the Oxygen Evolution Reaction. *ACS nano*, *18* (52), 35533–35549 (2024).
- Guo, M.; Dongfang, N.; Liu, Q.; Iannuzzi, M.; Bokhoven, J. A. van; Artiglia, L. Reaction Intermediates Involved in the Epoxidation of Ethylene Over Silver Revealed by In Situ Photoelectron Spectroscopy. *Small*, e2408432 (2024).
- Gäding, J.; Balda, V. D.; Lan, J.; Konrad, J.; Iannuzzi, M.; Meißner, R. H.; Tocci, G. The Role of the Water Contact Layer on Hydration and Transport at Solid/Liquid Interfaces. *Proc. Natl. Acad. Sci. United States Am.*, *121* (38), e2407877121 (2024).
- Bilichenko, M.; Iannuzzi, M.; Tocci, G. Slip Opacity and Fast Osmotic Transport of Hydrophobes at Aqueous Interfaces with Two-Dimensional Materials. *ACS Nano* (2024).
- Guo, M.; Dongfang, N.; Iannuzzi, M.; Bokhoven, J. A. van; Artiglia, L. Structure and Reactivity of Active Oxygen Species on Silver Surfaces for Ethylene Epoxidation. *ACS Catal.*, *14* (13), 10234–10244 (2024).
- Roithmeyer, H.; Bühler, J.; Blacque, O.; Tuncay, I.; Moehl, T.; Invernizzi, C.; Keller, F.; Iannuzzi, M.; Tilley, S. D. The Swiss Army Knife of Electrodes: Pillar[6]arene-Modified Electrodes for Molecular Electrocatalysis Over a Wide pH Range. *Angew. Chem. Int. Ed.*, e202413144 (2024).
- Folkestad, S. D.; Paul, A. C.; Paul, R.; Coriani, S.; Odelius, M.; Iannuzzi, M.; Koch, H. Understanding X-Ray Absorption in Liquid Water Using Triple Excitations in Multilevel Coupled Cluster Theory. *Nat. Commun.*, *15* (1), 3551 (2024).
- Roithmeyer, H.; Sévery, L.; Moehl, T.; Spingler, B.; Blacque, O.; Fox, T.; Iannuzzi, M.; Tilley, S. D. Electrocatalytic Ammonia Oxidation with a Tailored Molecular Catalyst Heterogenized via Surface Host–Guest Complexation. *J. Am. Chem. Soc.*, *146* (1), 430–436 (2024)
- Diulus, J. T.; Novotny, Z.; Dongfang, N.; Beckord, J.; Al-Hamdani, Y.; Comini, N.; Muntwiler, M.; Hengsberger, M.; Iannuzzi, M.; Osterwalder, J. H-BN/Metal-Oxide Interface Grown by Intercalation: A Model System for Nano-Confined Catalysis. *J. Phys. Chem. C* (2024).

2023

- Velasquez, N.; Nunes, F. B.; Travnikova, O.; Ismail, I.; Guillemin, R.; Martins, J. B.; Céolin, D.; Journel, L.; Fillaud, L.; Koulentianos, D.; Kamal, C.; Püttner, R.; Piancastelli, M. N.; Simon, M.; Odelius, M.; Iannuzzi, M.; Marchenko, T. X-Ray Induced Ultrafast Charge Transfer in Thiophene-Based Conjugated Polymers Controlled by Core-Hole Clock Spectroscopy. *Phys. Chem. Chem. Phys.* (2023).
- Dongfang, N.; Al-Hamdani, Y. S.; Iannuzzi, M. "Understanding the role of oxygen-vacancy defects in $Cu_2O(111)$ from first-principle calculations", *Electron. Struct. 5*, 035001(2023).
- Nunes, F. B.; Comini, N.; Diulus, J. T.; Huthwelker, T.; Iannuzzi, M.; Osterwalder, J.; Novotny, Z. "Dynamic Equilibrium at the HCOOH-Saturated TiO2(110)–Water Interface", *J Phys Chem Lett*, *14* (13), 3132–3138 (2023).
- Hutter, J.; Iannuzzi, M.; Kühne, T. D. "Ab Initio Molecular Dynamics: A Guide to Applications", *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*. (2023).
- Belleflamme, F.; Hehn, A.-S.; Iannuzzi, M.; Hutter, J., "A Variational Formulation of the Harris Functional as a Correction to Approximate Kohn-Sham Density Functional Theory", *J Chem Phys*, *158* (5), 054111 (2023).
- Sertcan, B.; Mousavi, S. J.; Iannuzzi, M.; Hamm, P. "Low-Frequency Anharmonic Couplings in Crystalline Bromoform: Theory" *J Chem Phys*, *158* (1), 014203 (2023).

2022

- Zhao, Y.; Wan, W.; Dongfang, N.; Triana, C. A.; Douls, L.; Huang, C.; Erni, R.; Iannuzzi, M.; Patzke, G. R. "Optimized NiFe-Based Coordination Polymer Catalysts: Sulfur-Tuning and Operando Monitoring of Water Oxidation", *ACS Nano, 16* (9), 15318–15327 (2022).
- Lan, J.; Iannuzzi, M. "Nuclear Quantum Effects at Aqueous Metal Interfaces Captured by Molecular Dynamics Simulations", *Curr Opin Electrochem*, *33*, 100934 (2022).
- Shao, F.; Wong, J. K.; Low, Q. H.; Iannuzzi, M.; Li, J.; Lan, J "In situ spectroelectrochemical probing of CO redox landscape on copper single-crystal surfaces", *Proc National Acad Sci* , 119, e2118166119 (2022).
- Melani, G.; Guerrero-Felipe, J. P.; Valencia, A. M.; Krumland, J.; Cocchi, C.; Iannuzzi, M. "Donors, Acceptors, and a Bit of Aromatics: Electronic Interactions of Molecular Adsorbates on hBN and MoS 2 Monolayers", *Phys Chem Chem Phys*, *24* (27), 16671–16679 (2022).

- Zhao, Y.; Dongfang, N.; Triana, C. A.; Huang, C.; Erni, R.; Wan, W.; Li, J.; Stoian, D.; Pan, L.; Zhang, P.; Lan, J.; Iannuzzi, M.; Patzke, G. R. "Dynamics and Control of Active Sites in Hierarchically Nanostructured Cobalt Phosphide/Chalcogenide-Based Electrocatalysts for Water Splitting", *Energ Environ Sci*, 15 (2), 727–739 (2022).
- Herrero, C.; Pauletti, M.; Tocci, G.; Iannuzzi, M.; Joly, L. "Connection between Water's Dynamical and Structural Properties: Insights from Ab Initio Simulations" *Proc National Acad Sci*, 119 (21), e2121641119 (2022).
- Pauletti, M., Rybkin, V. V., Iannuzzi, M., "Surface tension of liquids and binary mixtures from molecular dynamics simulations", *J Phys Condens Matter*, 34, 044003 (2022).

2021

- Pauletti, M,; Rybkin, V.V.; Iannuzzi, M., "Subsystem Density Functional Theory Augmented by a Delta Learning Approach to Achieve Kohn–Sham Accuracy", *J. Chem. Theory Comput.*, 17, 6423–6431 (2021).
- Reinholdt, P., M. L. Vidal, J. Kongsted, Iannuzzi, M.; Coriani, S.; Odelius, M., "Nitrogen K-Edge X-ray Absorption Spectra of Ammonium and Ammonia in Water Solution: Assessing the Performance of Polarizable Embedding Coupled Cluster Methods", *J Phys Chem Lett*, 12, 8865-8871 (2021).
- Joly, L.; Meissner, R. H.; Iannuzzi, M.; Tocci, G., "Osmotic Transport at the Aqueous Graphene and hBN Interfaces: Scaling Laws from a Unified, First-Principles Description", *Acs Nano* 15, 15249-5258 (2021).
- Le, Jia-Bo; Chen, Ao; Li, Lang; Xiong, Jing-Fang; Lan, Jinggang; Liu, Yun-Pei; Iannuzzi, Marcella; Cheng, Jun, "Modeling Electrified Pt(111)-Had/Water Interfaces from Ab Initio Molecular Dynamics", *JACS Au*, 1, 569–577 (2021).
- Savchenko, V.; Brumboiu, I. E.; Kimberg, V.; Odelius, M.; Krasnov, P.; Liu, J.-C.; Rubensson, J.-E.; Björneholm, O.; Sathe, C.; Grasjö, J.; Dong, M.; Pietzsch, A.; Föhlisch, A.; Schmitt, T.; McNally, D.; Lu, X.; Polyutov, S. P.; Norman, P.; Iannuzzi, M.; Gelmukhanov, F.; Ekholm, V., "Vibrational Resonant Inelastic X-Ray Scattering in Liquid Acetic Acid: A Ruler for Molecular Chain Lengths", *Scientific Reports*, 11, 4098 (2021).
- Baumann, N.; Lan, J.; Iannuzzi, M., "CO_2 adsorption on the pristine and reduced CeO_2 (111) surface: Geometries and vibrational spectra by first principles simulations", *Journal Chemical Physics*, 154, 094702 (2021).
- Severy, L.; Szczerbinski, J.; Taskin, M.; Tuncay, I.; Nunes, F. B.; Cignarella, C.; Tocci, G.; Blacque, O.; Osterwalder, J.; Zenobi, R.; Iannuzzi, M.; Tilley, S. D., "Immobilization of molecular catalysts on electrode surfaces using host-guest interactions", *Nature Chemistry*, 13, 523–529 (2021).
- Lan, J,; Kapil, V.; Gasparotto, P.; Ceriotti, M.; Iannuzzi, M.; Rybkin, V.V., "Simulating the Ghost: Quantum Dynamics of the Solvated Electron ", *Nature Communication*, 12, 766 (2021).
- Wilks, R. G.; Erbing, A.; Sadoughi, G.; Starr, D. E.; Handick, E.; Meyer, F.; Benkert, A.; Iannuzzi, M.; Hauschild, D.; Yang, W.; Blum, M.; Weinhardt, L.; Heske, C.; Snaith, H. J.; Odelius, M.; Bär, M., "Dynamic Effects and Hydrogen Bonding in Mixed-Halide Perovskite Solar Cell Absorbers", *J Phys Chem Lett*, 12, 3885–3890 (2021).

2020

- Cun, H.; Miao, Z.; Hemmi, A.; Al-Hamdani, Y.; Iannuzzi, M.; Osterwalder, J.; Altman, M. S.; Greber, T., "High- Quality Hexagonal Boron Nitride from 2D Distillation", *Acs Nano*, 15 , 1351–1357 (2020).
- Gurdal, Y.; Iannuzzi, M., "Comparison of Penta and Tetra-pyridyl Cobalt-based Catalysts for Water Reduction: H_2 Production Cycle, Solvent Response and Reduction Free Energy", *Chemphyschem*, 21, 1–10 (2020).
- Algarra, A. G.; Burnage, A. L.; Iannuzzi, M.; Krämer, T.; Macgregor, S. A.; Pirie, R. E. M.; Tegner, B.; Weller, A. S., "Computational Studies of the Solid-State Molecular Organometallic (SMOM) Chemistry of Rh σ-Alkane Complexes", *In Structure and Bonding; Springer, Ed.; Springer Berlin Heidelberg: Berlin, Heidelberg*, 181, 1–46 (2020).
- Wan, W.; Triana, C. A.; Lan, J.; Li, J.; Allen, C. S.; Zhao, Y.; Iannuzzi, M.; Patzke, G. R., "Bifunctional Single Atom Electrocatalysts: Coordination-Performance Correlations and Reaction Pathways", *Acs Nano*, 14, 13279–13293 (2020).
- Kühne, T. D.; Iannuzzi, M.; Ben, M. D.; Rybkin, V. V.; Seewald, P.; Stein, F.; Laino, T.; Khaliullin, R. Z.; Schütt, O.; Schiffmann, F.; Golze, D.; Wilhelm, J.; Chulkov, S.; Bani-Hashemian, M. H.; Weber, V.; Borstnik, U.; Taillefumier, M.; Jakobovits, A. S.; Lazzaro, A.; Pabst, H.; Müller, T.; Schade, R.; Guidon, M.; Andermatt, S.; Holmberg, N.; Schenter, G. K.; Hehn, A.; Bussy, A.; Belleflamme, F.; Tabacchi, G.; Gloss, A.; Lass, M.; Bethune, I.; Mundy, C. J.; Plessl, C.; Watkins, M.; VandeVondele, J.; Krack, M.; Hutter, J., "CP2K: An Electronic Structure and Molecular Dynamics Software Package − Quickstep: Efficient and Accurate Electronic Structure Calculations", *J. Chemical Physics*, 152, 194103 (2020).
- Lan, J.; Rybkin, V.V.;Iannuzzi, M.,"Ionization of Water as an Effect of Quantum Delocalization at Aqueous Electrode Interfaces", *J. Physical Chemistry Letters*, 11, 3724-3730 (2020).

- Tocci, G.; Bilichenko, M.; Joly, L.; Iannuzzi, M., "Ab initio Nanofluidics: Disentangling the role of the energy landscape and of density correlations on liquid/solid friction", *Nanoscale*, 12, 10994–1100 (2020).

2019

- Alberto, R.; Iannuzzi, M.; Gurdal, Y.; Probst, B., "[CoII(BPyPy$_2$COH)(OH$_2$)$_2$]$^{2+}$: A Catalytic Pourbaix Diagram and AIMD Simulations on Four Key Intermediates" , *Chimia*, 73, 906–912 (2019).
- Kliuiev, P.; Zamborlini, G.; Jugovac, M.; Gurdal, Y.; Arx, K. von; Waltar, K.; Schnidrig, S.; Alberto, R.; Iannuzzi, M.; Feyer, V.; Hengsberger, M.; Osterwalder, J.; Castiglioni, L., "Combined orbital tomography study of multi- configurational molecular adsorbate systems", *Nature Communications*, 10, 5255 (2019).
- Zabka, W.-D.; Musso, T.; Mosberger, M.; Novotny, Z.; Totani, R.; Iannuzzi, M.; Probst, B.; Alberto, R.; Osterwalder, J., "Comparative study of the different anchoring of organometallic dyes on ultrathin alumina", *Journal of Physical Chemistry C* 123(36), 22250–22260 (2019).
- Hemmi, A.; Cun, H.; Tocci, G.; Epprecht, A.; Stel, B.; Lingenfelder, M.; Lima, L. H. de; Muntwiler, M.; Osterwalder, J.; Iannuzzi, M.; Greber, T., "Catalyst Proximity-Induced Functionalization of h-BN with Quat Derivatives", *Nano Letters* 19(9), 5998–6004 (2019).
- The PLUMED consortium, "Promoting transparency and reproducibility in enhanced molecular simulations", *Nature Methods* 16, 670–673 (2019).
- Foppa, L.; Iannuzzi, M.; Copèret, C.; Comas-Vives, A., "Facile Fischer-Tropsch Chain Growth from CH_2 Monomers Enabled by the Dynamic CO Adlayer", *ACS Catalysis* 9, 6571–6582 (2019).
- Wick-Joliat, R.; Musso, T.; Prabhakar, R. R.; Löckinger, J.; Siol, S.; Cui, W.; Severy, L.; Moehl, T.; Suh, J.; Hutter, J.; Iannuzzi, M.; Tilley, S. D., "Stable and tunable phosphonic acid dipole layer for band edge engineering of photoelectrochemical and photovoltaic heterojunction devices", *Energy Environmental Science* 12, 1901–1909.(2019).
- Cruz, V. V. da; Gelmukhanov, F.; Eckert, S.; Iannuzzi, M.; Ertan, E.; Pietzsch, A.; Couto, R. C.; Niskanen, J.; Fondell, M.; Dantz, M.; Schmitt, T.; Lu, X.; McNally, D.; Jay, R. M.; Kimberg, V.; Föhlisch, A.; Odelius, M., "Probing hydrogen bond strength in liquid water by resonant inelastic X-ray scattering" *Nature Communications* 10(1), 1013 (2019).
- Foppa, L.; Iannuzzi, M.; Copèret, C.; Comas-Vives, A., "CO methanation on ruthenium flat and stepped surfaces: Key role of H-transfers and entropy revealed by ab initio molecular dynamics", *Journal of Catalysis* 371, 270–275 (2019).

2018

- Staub, R.;Iannuzzi, M.; Khaliullin, R.Z.; Steinmann, S.,"Energy Decomposition Analysis for Metal Surface-Adsorbate Interactions by Block Localized Wave Functions", *Journal of Chemical Theory and Computation* 15(1), 265–275 (2018).
- Lan, J.; Hutter, J.; Iannuzzi, M., "First-Principles Simulations of an Aqueous CO/Pt(111) Interface", *Journal of Physi- cal Chemistry C* 122, 24068–24076 (2018).
- Silva, C. C.; Iannuzzi, M.; Duncan, D. A.; Ryan, P. T. P.; Clarke, K. T.; Küchle, J. T.; Cai, J.; Jolie, W.; Schlueter, C.; Lee, T.-L.; Busse, C., "Valleys and Hills of Graphene on Ru(0001)", *Journal of Physical Chemistry C* 122, 18554– 18561 (2018).
- Foppa, L.; Iannuzzi, M.; Copèret, C.; Comas-Vives, A., "Adlayer Dynamics Drives CO Activation in Ru-Catalyzed Fischer-Tropsch Synthesis", *ACS Catalysis* 8, 6983–6992 (2018).
- Musso, T.; Caravati, S.; Hutter, J.; Iannuzzi, M.,"Second generation Car-Parrinello MD: application to the h-BN/Rh(111) nanomesh", *European Physical Journal B* 91, 148 (2018).
- Steinmann, S. N.; Morais, R. F. D.; Götz, A. W.; Fleurat-Lessard, P.; Iannuzzi, M.; Sautet, P.; Michel, C., "Force Field for Water over Pt(111): Development, Assessment, and Comparison", *Journal of Chemical Theory and Computation* 14, 3238–3251 (2018).
- Palecek, D.; Tek, G.; Lan, J.; Iannuzzi, M.; Hamm, P., "Characterization of the Platinum-Hydrogen Bond by Surface- Sensitive Time-Resolved Infrared Spectroscopy", *Journal of Physical Chemistry Letters* 9, 1254–1259 (2018).
- Mondal, A.; Gaultois, M. W.; Pell, A. J.; Iannuzzi, M.; Grey, C. P.; Hutter, J.; Kaupp, M., "Large-Scale Computa- tion of Nuclear Magnetic Resonance Shifts for Paramagnetic Solids Using CP2K", *Journal of Chemical Theory and Computation* 14, 377–394 (2018).
- Müller, R.J.; Lan, J.; Lienau, K.; Moré, R.; Triana, C.A.; Iannuzzi, M.; Patzke, G.R., "Monitoring surface transformations of metal carbodiimide water oxidation catalysts by operando XAS and Raman spectroscopy", *Dalton Transactions* 47, 10759–10766 (2018).

2017

- Ekimova, M.; Quevedo, W.; Szyc, L.; Iannuzzi, M.; Wernet, P.; Odelius, M.; Nibbering, E. T. J., "Aqueous Solvation of Ammonia and Ammonium: Probing Hydrogen Bond Motifs with FT-IR and Soft X-ray Spectroscopy", *Journal of the American Chemical Society*, 139(36), 12773–12783 (2017).
- Eckert, S.; Niskanen, J.; Jay, R. M.; Miedema, P. S.; Fondell, M.; Kennedy, B.; Quevedo, W.; Iannuzzi, M.; Fhlisch, A., "Valence orbitals and local bond dynamics around N atoms of histidine under X-ray irradiation", *Physical Chemistry Chemical Physics* 19(47), 32091-32098 (2017).
- Le, J.; Iannuzzi, M.; Cuesta, A.; Cheng, J., "Determining Potentials of Zero Charge of Metal Electrodes versus the Standard Hydrogen Electrode from Density-Functional-Theory-Based Molecular Dynamics", *Physical Review Letters* 119, 016801 (2017).
- Graf, M.; Mette, G.; Leuenberger, D.; Gurdal, Y.; Iannuzzi, M.; Zabka, W.-D.; Schnidrig, S.; Probst, B.; Hutter, J.; Alberto, R.; Osterwalder, J., "The impact of metalation on adsorption geometry, electronic level alignment and UV-stability of organic macrocycles on TiO_2(110)", *Nanoscale* 9, 8756–8763 (2017).
- Kachmar, A.; Carignano, M.; Laino, T.; Iannuzzi, M.; Hutter, J., "Mapping the free energy of lithium solvation in the protic ionic liquid Ethylammonuim Nitrate: A metadynamics study", *ChemSusChem* (2017).
- Barman, S.; Remhof, A.; Koitz, R.; Iannuzzi, M.; Blacque, O.; Yan, Y.; Fox, T.; Hutter, J.; Zttel, A.; Berke, H., "Post-synthesis amine borane functionalization of metal-organic framework and its unusual chemical hydrogen release phenomenon", *Chemistry: a European Journal* 23, 1–7 (2017).
- Gurdal, Y.; Hutter, J.; Iannuzzi, M., "Insight into (Co)Pyrphyrin Adsorption on Au(111): Effects of Herringbone Reconstruction and Dynamics of Metalation", *Journal of Physical Chemistry C* (2017).
- Golze, D.; Iannuzzi, M.; Hutter, J., "Local Fitting of the Kohn–Sham Density in a Gaussian and Plane Waves Scheme for Large-Scale Density Functional Theory Simulations", *Journal of Chemical Theory and Computation* 13, 2202–2214 (2017).
- Ertan, E.; Kimberg, V.; Gelmukhanov, F.; Hennies,F .; Rubensson, J.E.; Schmitt, T.; Strocov, V.N.; Zhou, K.; Iannuzzi, M.; Föhlisch, A.; Odelius, M.; Pietzsch, A., "Theoretical simulations of oxygen K-edge resonant inelastic x-ray scattering of kaolinite", *Phyical Review B* 95, 144301 (2017).
- Golze, D.; Benedikter, N.; Iannuzzi, M.; Wilhelm, J.; Hutter, J., "Fast evaluation of solid harmonic Gaussian integrals for local resolution-of-the-identity methods and range-separated hybrid functionals", *Journal of Chemical Physics* 146, 034105 (2017).
- Ré ocreux, R.; Jiang, T.; Iannuzzi, M.; Michel, C.; Sautet, P., "Structuration and Dynamics of Interfacial Liquid Water at Hydrated γ-Alumina Determined by Ab Initio Molecular Simulations: Implications for Nanoparticle Stability", *Applied Nano Materials*, 1, 191–199 (2017).
- Gurdal, Y., Iannuzzi, M., "DFT-based theoretical simulations for photocatalytic applications using TiO_2", in: *Titan. Dioxide*, InTech, (2017).

2015-2016

- Lanzani, G.; Seitsonen, A. P.; Iannuzzi, M.; Laasonen, K.; Pehkonen, S. O., "Isomerism of Trimeric Aluminum Com- plexes in Aqueous Environments: Exploration via DFT-Based Metadynamics Simulation", *Journal of Physical Chemistry B* 120, 11800–11809 (2016).
- Sala, O.; Santschi, N.; Jungen, S.; Lu ̈thi, H. P.; Iannuzzi, M.; Hauser, N.; Togni, A., "S-Trifluoromethylation of Thiols by Hypervalent Iodine Reagents: A Joint Experimental and Computational Study", *Chem. Eur. J.* 22, 1704–1713 (2016).
- Chadwick, F. M.; Rees, N. H.; Weller, A. S.; Kra ̈mer, T.; Iannuzzi, M.; Macgregor, S. A. A., "A Rh-pentane sigma- alkane complex. Characterization in the solid-state by experimental and computational techniques", *Angewandte Chemie International Edition*, 55, 3677–3681 (2016).
- Koitz,R.;Hutter,J.;Iannuzzi,M.,"FormationandPropertiesofaTerpyridine-based2DMOFontheSurfaceofWater", *2D Materials* 3, 025026 (2016).
- Mette, G.; Sutter, D.; Gurdal, Y.; Schnidrig, S.; Probst, B.; Iannuzzi, M.; Hutter, J.; Alberto, R.; Osterwalder, J., "From porphyrins to pyrphyrins: Adsorption study and metalation of a molecular catalyst on Au(111)", *Nanoscale* 8, 7958–7968 (2016).
- Y. Guerdal, S. Luber, J. Hutter, M. Iannuzzi, "Non-innocent adsorption of Co-pyrphyrin on rutile(110)" *Physical Chemistry Chemical Physics* 17, 22846-22854 (2015).
- M. Pré mont-Schwarz, S. Schreck, M. Iannuzzi, E.T.J. Nibbering, M. Odelius, P. Wernet, "Correlating Infrared and X- ray Absorption Energies for Molecular-Level Insight into Hydrogen Bond Making and Breaking in Solution" *Journal of Physical Chemistry B* 119(25), 8115-8124 (2015).
- M. Iannuzzi, "Ar Implantation at the hBN/Rh(111) Nanomesh by ab Initio Molecular Dynamics" *Journal of Physical Chemistry C* 119(38), 22198-22207 (2015).
- J. Sgrignani, M. Iannuzzi, A. Magistrato, "Role of Water in the Puzzling Mechanism of the Final Aromatization Step Promoted by the Human Aromatase Enzyme. Insights from QM/MM MD Simulations" *Journal of Chemical Informa- tion and Modeling* 55(10), 2218–2226 (2015).

- O. Sala, H.P. Luthi, A. Togni, M. Iannuzzi, J. Hutter, "Dividing a complex reaction involving a hypervalent iodine reagent into three limiting mechanisms by ab initio molecular dynamics" *J. Comput. Chem.* 36(11), 785–794 (2015).
- A. Lunghi, M. Iannuzzi, R. Sessoli, F. Totti, "Evolution of Structural and Magnetic Properties of the Single Molecule Magnets Fe4C5 grafted on Au(111) from Ab Inition Molecular Dynamics.", *J. Mat. Chem. C* (2015).
- R. Koitz, M. Iannuzzi, J. Hutter, "Building Blocks for Two-Dimensional Metals- Organic Frameworks Confined at the Air-Water Interface: An Ab Initio Molecular Dynamics Study", *J. Phys. Chem. C* 119(8), 4023–4030 (2015).
- K. Hahn, M. Iannuzzi, A.P. Seitsonen, J. Hutter, "Functionalization of CeO_2(111) by Deposition of Small Ni Clusters: Effects on CO_2 Adsorption and O Vacancy Formation", *ChemCatChem*, 7(4), 706 (2015).
- H. Cun, M. Iannuzzi, A. Hemmi, J. Osterwalder, T. Greber "Ar implantation beneath graphene on Ru(0001): Nanotents and can-opener effect", *Surface Science* 634, 95–102 (2015).
- D. Golze, J. Hutter, M. Iannuzzi, "Wetting of water on hexagonal boron nitride @Rh(111): A QM/MM model based on atomic charges derived for nano-structured surfaces", *PCCP* 17(22), 14307–14316 (2015).
- L. Weinhardt, E. Ertan, M. Iannuzzi, M. Weigand, O. Fuchs, M. Bär, M. Blum, J.D. Denlinger, W. Yang, E. Umbach, M. Odelius, C. Heske " Probing hydrogen bonding orbitals: resonant inelastic soft X-ray scattering of aqueous NH_3" *PCCP* 17(40), 27145–27153 (2015).

2013-2014

- T. Dienel, J. Gomez-Diaz, A. P. Seitsonen, R. Widmer, M. Iannuzzi, K. Radican, H. Sachdev, K. Mu¨llen, J. Hutter, O. Gröning, "Dehalogenation and Coupling of Polycyclic Hydrocarbon on an Atomically Thin Insulator", *ACS Nano*, (2014).
- D. Adams, S. Chappellet, F. Lincker, M. Ibn-Elhaj, B. Watts, M. Iannuzzi, D. Sisak, C. Pignedoli, D. Passerone, "Identifying Photoreaction Products in Cinnamate Based Photoalignment Materials", *J Phys Chem C*, (2014).
- M. Iannuzzi, F. Tran, R. Widmer, T. Dienel, K. Radican, Y. Ding, J. Hutter, O. Gro¨ning, "Site-selective adsorption of phthalocyanine on h-BN/Rh(111) nanomesh", *PCCP*, 16, 12374 (2014).
- H. Cun, M. Iannuzzi, A. Hemmi, J. Osterwalder, T. Greber, "2 nm Voids in Single Layer Hexagonal Boron Nitride: Formation by "Can-opener" Effect and Annihilation by Self-healing", *ACS Nano*, 8, 7423–7431 (2014).
- S. Luber, M. Iannuzzi, J. Hutter, "Raman spectra from ab initio molecular dynamics and its application to liquid S- Methyloxirane", *J. Chem. Phys.*, 7, 094503 (2014).
- S. Barman, A. Khutia, R. Koitz, O. Blacque, H. Furukawa, M. Iannuzzi, J. Hutter, O. M. Yaghi, C. Janiak, H. Berke, "Synthesis and hydrogen adsorption properties of internally polarized 2,6-azulenedicarboxylate based MOFs", *J. Mater. Chem. A*, 2, 18823–18830 (2014).
- P. Bacle, A. P. Seitsonen, M. Iannuzzi, J. Hutter, "Chemical Reactions on Metal-Supported Hexagonal Boron Nitride Investigated with Density Functional Theory", *Chimia*, (2014).
- J. Hutter, M. Iannuzzi, F. Schiffmann, J. Vande Vondele,"CP2K: Atomistic Simulations of Condensed Matter Systems.", Wiley Interdisciplinary Reviews: Computational Molecular Science Article, 4(1), 15–25 (2014).
- K. Hahn, M. Iannuzzi, A. Seitsonen, J. Hutter, "Coverage effect of the CO_2 adsorption mechanisms on CeO_2(111) by first principles analysis", *J Phys Chem C*, 117, 1701 (2013).
- F. Totti, G. Rajaraman, M. Iannuzzi, R. Sessoli, "Computational Studies on SAMs of Mn6 SMMs on Au(111): Do properties change upon grafting?", *J Phys Chem C*, 117(14), 7186–7190 (2013).
- J. Go´mez D´ıaz, Y. Ding, R. Koitz, A.P. Seitsonen, M. Iannuzzi, J. Hutter, "Hexagonal Boron Nitride on Transition Metal Surfaces", *Theor Chem Acc*, 132, 1350 (2013).
- M. Iannuzzi, I. Kalichava, H. Ma, S.J. Leake, H. Zhou, G. Li, Y. Zhang, O. Bunk, H. Gao, P. Willmot, J. Hutter, T. Greber, "Moire beatings in graphene on Ru(0001) superstructure.", *Phys. Rev. B*, 88, 125433 (2013).
- H. Cun, M. Iannuzzi, A. Hemmi, S. Roth, J. Osterwalder, T. Greber, "Immobilizing Individual Atoms beneath a Cor- rugated Single Layer of Boron Nitride ", *Nano Lett.*, 13(5), 2098–2103 (2013).
- R. Koitz, A.P. Seitsonen, M. Iannuzzi, J. Hutter, "Structural and Electronic Properties of a Large-Scale Moire´ Pattern of Hexagonal Boron Nitride on Cu(111) Studied with Density Functional Theory", *Nanoscale*, 5(12), 5589–5595 (2013).
- D. Golze, M. Iannuzzi, M. Nguyen, D. Passerone, J. Hutter, "Simulation of adsorption processes at metallic interfaces: An image charge-augmented QM/MM approach", *J. Chem. Theo. Comp.*, 9, 5086 (2013).
- H. Cun, M. Iannuzzi, A. Hemmi, J. Osterwalder, T. Greber, "Implantation Length and Thermal Stability of Interstitial Ar Atoms in Boron Nitride Nanotents", *ACS Nano*, 8, 1014–1021 (2013).

2010-2012

- M.L. Bonnet, M. Iannuzzi, D. Sebastiani, J. Hutter, "Local Disorder in Lithium Imide from First principles simulation and NMR Spectroscopy ", *J. Phys. Chem. C*, 116, 18577 (2012).
- J.L. Valles Pardo, M. Guijt, M. Iannuzzi, S.K. Joya, H.J.M. de Groot, F. Buda, "Ab-initio molecular dynamics study of water oxidation reaction pathways in mono-Ru catalysts", *ChemPhysChem*, 13, 140 (2012).
- H. Ma, Y. Ding, M. Iannuzzi, T. Brugger, S. Berner, J. Hutter, J. Osterwalder, T. Greber, "Chiral distortion of confined ice oligomers (N = 5,6)", *Langmuir*, 28, 15246 (2012).
- Y. Ding, M. Iannuzzi, J. Hutter, "Possible models for nono-ice structures formed in the pore of the hBN/Rh nanomesh", *J Phys Condens Matter*. 24, 445002 (2012).
- F. Devybck, M. Iannuzzi, M. Krack, "Frenkel pair recombinations in UO_2: Importance of explicit description of polarizability in core-shell molecular dynamics simulations", *Phys. Rev. B*, 85, 184103 (2012).
- S. Joshi, D. Ecija, R. Koitz, M. Iannuzzi, A.P. Seitsonen, J. Hutter, H. Sachdev, S. Vijayaraghavan, F. Bischoff, K. Seufert, J.V. Barth, W. Auwärter, "Boron nitride on Cu(111): An electronically corrugated monolayer", *Nano Lett.*, 12, 5821 (2012).
- Y. Ding, M. Iannuzzi, J. Hutter, "Investigation of Boron Nitride Nanomesh Interacting with Water", *J. Physical Chemitry C*, 115(28), 13685–13692 (2011).
- Y. Ding, M. Iannuzzi, J. Hutter, "Investigation of h-BN/Rh(111) Nanomesh Interacting with Water and Atomic Hydrogen", *Chimia*, 65 (4), 256 (2011).
- M. Iannuzzi, J. Hutter, " Comparative study of the nature of chemical bonding of corrugated graphene on Ru(0001) and Rh(111) by electronic structure calculation", *Surface Science*, 605, 1360–1368 (2011).
- G.Santarossa,A.Vargas,M.Iannuzzi,A.Baiker,"Free energy surface of two-and three-dimensional transitions of Au12 nanoclusters obtained by ab initio metadynamics", 81 (17), 174205 (2010).
- T. Brugger, H. Ma, M. Iannuzzi, S. Berner, A. Winkler, J. Hutter, J. Osterwalder, T. Greber, "Nanotexture Switching of Single-Layer Hexagonal Boron Nitride on Rhodium by Intercalation of Hydrogen Atoms", *Angew Chem Int Edit*, 49(35), 6120–6124 (2010).

Until 2009

- H. Ma, T. Brugger, S. Berner, Y. Ding, M. Iannuzzi, J. Hutter, J. Osterwalder, T. Greber,"Nano-ice on Boron Nitride Nanomesh: Accessing Proton Disorder", *ChemPhysChem*, 11 (2), 399–403 (2010).
- V. Weber, M. Iannuzzi, S. Giani, J. Hutter, R. Declerck, M. Waroquier, "Magnetic linear response properties calcula- tions with the Gaussian and augmented-plane-wave method", *J. Chem. Phys.*, 131 (1) 014106 (2009).
- A.Vargas, G. Santarossa, M. Iannuzzi, A. Baiker,"Fluxionality of gold nanoparticles investigated by Born-Oppenheimer molecular dynamics.", *Phys. Rev. B*, 80(19), 195421 (2009).
- A. Vargas, G. Santarossa, M. Iannuzzi, and A. Baiker, "Chiral recognition on catalytic surfaces: Theoretical insight in a bio-mimetic heterogeneous catalytic system", *J. Phys. Chem. C*, (2008).
- C. Mundy, A. Curioni, I-F.W. Kuo, E.J. Reed and M. Iannuzzi, "Ultrafast transformation of graphite to diamond: An ab-initio study of graphite under shock compression", *J. Chem. Phys.*, 128, 184701 (2008).
- M.Iannuzzi, "X-ray absorption spectra of hexagonal ice and liquidwater by all-electron Gaussian and augmented plane wave calculations", *J. Chem. Phys.*, 128, 204506 (2008).
- A. Rodriguez-Fortea, M. Iannuzzi, "First-Principles Molecular Dynamics Study of the Heterogeneous Reduction of NO_2 on Soot Surfaces", *J. Phys. Chem. C*, 112(49), 19642 (2008).
- A. Vargas, G. Santarossa, M. Iannuzzi, A. Baiker, "Chiral recognition on catalytic surfaces: Theoretical insight in a biomimetic heterogeneous catalytic system", *J. Phys. Chem. C*, 112(27), 10200 (2008).
- G. Santarossa, C. Pignedoli, A. Vargas, M. Iannuzzi, D. Passerone, A. Baiker, "Modeling bulk and surface Pt using the "Gaussian and plane wave" density functional theory formalism: Validation and comparison to k-point plane wave calculations.", *J. Chem. Phys.*, 129(23) 234703 (2008).
- A. Rodriguez-Fortea, M. Iannuzzi, M. Parrinello, "Ab initio molecular dynamics study of heterogeneous nitric acid decomposition reactions on graphite surfaces", *J. Phys. Chem. C*, 111(5), 2251–2258 (2007).
- A. Urakawa, M. Iannuzzi, J. Hutter, and A. Baiker, "Carbon Dioxide Hydrogenation Catalyzed by Ruthenium Dihydride: Ab Initio Metadynamics Investigation", *Chem. Eur J.*, 13(24), 6828–6480 (2007).
- M. Iannuzzi, J. Hutter, "Inner-shell spectroscopy by the Gaussian and augmented plane wave method", *Phys. Chem. Chem. Phys.*, 9(13), 1599–1610 (2007).
- M. Iannuzzi, "Proton Transfer in Imidazole Based Molecular Crystals", *J. Chem. Phys.*, 124(20), 204710 (2006).
- M. Pagliai, M. Iannuzzi, G. Cardini, M. Parrinello, and V. Schettino, "Lithium Hydroxide Phase Transition under High Pressure: an ab-initio Molecular Dynamics Study", *ChemPhysChem*, 7(1), 141-147 (2006).

- A. Rodriguez-Fortea, M. Iannuzzi, and M Parrinello, "Ab-Initio Molecular Dynamics Study of Heterogeneous Oxidation of Graphite by Means of Gas Phase Nitric Acid", *J. Phys. Chem. B*, 110(8), 3477-3484 (2006).
- M. Iannuzzi, B. Kirchner, and J. Hutter, "Density Functional Embedding for Molecular Systems ", *Chem. Phys. Lett.*, 421(1-3), 16–20 (2006).
- J. VandeVondele, M. Iannuzzi, and J. Hutter, "Large scale condensed matter calculations using the gaussian augmented plane waves method", *Lect. Notes Phys.*, 703, 287–314, Springer-Verlag Berlin Heidelberg (2006).
- J. Park, A. Laio, M. Iannuzzi, and M. Parrinello, "Dissociation Mechanism of an Acetic Acid in Water", *J. Am. Chem. Soc.*, 128(35), 11318-11319 (2006).
- J. Hutter and M. Iannuzzi, "CPMD: Car-Parrinello Molecular Dynamics", *Zeitschrift für Christallographie*, 220, 549 (2005).
- A. Stirling, M. Iannuzzi, M. Parrinello, F. Molnar, V. Bernhart, and G.A. Luinstra, "β -Lactone Synthesis from Epoxide and CO: Reaction Mechanism Revisited", *Organometallics*, 24, 2533 (2005).
- M. Iannuzzi, T. Chassaing, and J. Hutter, "Ground and Excited State density Functional Calculations with Gaussian and Augmented Plane Waves Method", *Chimia*, 59(7-8), 499–503 (2005).
- A. Stirling, M. Iannuzzi, A. Laio, and M. Parrinello, "Azulene-to-Naphthalene Rearrangement: The Car-Parrinello Metadynamics Method Explores Various Reaction Mechanisms", *ChemPhysChem*, 5, 1558 (2004).
- M. Iannuzzi and M. Parrinello, "Proton transfer in heterocycle crystals", *Phys. Rev. Lett.* , 93, 025901 (2004).
- S. Churakov, M. Iannuzzi, and M. Parrinello, "Ab-initio study of dehydroxylation carbonation reaction on brucite surface", *J. Phys. Chem. B*, 108, 11567 (2004).
- F.L. Gervasio, A. Laio, M. Iannuzzi, and M. Parrinello, "Influence of DNA structure on the reactivity of the guanine radical cation", *Chemistry-A Eur. J.*, 10, 4846 (2004).
- M. Iannuzzi, A. Laio, M. Parrinello, "Reactive Car-Parrinello molecular dynamics", *Phys. Rev. Lett.*, 90 238302 (2003).
- M. Iannuzzi and M. Parrinello, "Wavefunction localization in reciprocal space", *Phys. Rev. B*, 66, 155209 (2002).
- M. Iannuzzi P. Raiteri, M. Celino and L. Miglio, "Point defects and stacking faults in $TiSi_2$ phases by tight binding molecular dynamics", *J. Phys: Condens. Matter*, 14, 9535 (2002).
- M. Iannuzzi, P. Raiteri and L. Miglio, "Self-diffusion of silicon in $TiSi_2$ competing phases by tight binding molecular dynamics", *Computational Materials Science*, 20, 394, 2001.
- L. Miglio, M. Iannuzzi, P. Raiteri, M. Celino, "Silicon diffusion in competitive $TiSi_2$ phases by molecular dynamics simulations", *Microelectronic Engineering*, 55, 83, 2001.
- M. Iannuzzi and L. Miglio, "Surface energies and surface relaxation at $TiSi_2$ competing phases", *Surface Science* , 479 , 201 (2001).
- M. Iannuzzi and M. Parrinello, "Efficient k · p method for the calculation of total energy and electronic density of states", *Phys. Rev. B*, 64, 233104 (2001).
- F. LaVia, V. Ranieri, M.G. Grimaldi, L. Miglio, M. Iannuzzi, F. Marabelli, S. Bocelli, S. Santucci and A.R. Phani, "Role of substrate in the *c*49−*c*54 transformation of $TiSi_2$", *J. of Vacuum. Sci. Tecn. B*, 18, 721, (2000).
- M. Iannuzzi, L. Miglio and M. Celino, "Structural and thermoelastic properties of crystalline and amorphous $TiSi_2$ phases by tight binding molecular dynamics", *Phys. Rev. B*, 61, 14405, 2000.
- L. Miglio, M. Iannuzzi, M.G. Grimaldi, F. La Via, F. Marabelli, S. Bocelli, S. Santucci and A.R. Phani "Texturing, surface energetics and morphology in *c*49 − *c*54 transformation of $TiSi_2$ ", *Solid-State Electronics*, 43, 1069, (1999).
- L. Miglio, M. Iannuzzi, M. Celino, R. Pastorelli, C. Bottani, A. Sabbadini and G. Pavia, "Supersoft elastic parameters and low melting temperature of the *c*49 phase in $TiSi_2$ by Brillouin scattering and molecular dynamics", *Appl. Phys. Lett.*, 74, 3654, (1999).
- F.Bonoli, M.Iannuzzi L.Miglio and V.Meregalli "Electronic origin of the stability trend in $TiSi_2$ phases with Al or Mo layers", *Appl. Phys. Lett.*, 73, 1964, (1998).
- M.G.Grimaldi, F.LaVia, V.Raineri, S.Bocelli, M.Galli, F.Marabelli, F.Bonoli, M.Iannuzzi and L.Miglio, "Kinetics of the *c*49−*c*54 phase transition in $TiSi_2$: new indications from sheet resistance, infrared spectroscopy and molecular dynamics simulations", *Microelectronic Engineering*, 37-38, 443, (1997).

Contributions to international conferences in the past four years

28/01/2025: Molecular and Electronic Dynamics at Different Time Scales by Density Functional Theory**,** Swiss Association of Computational Chemistry Spring Meeting 2025, Bern

18/06/2024: *Hydration and Transport at Solid/Liquid Interfaces by ab initio Molecular Dynamics*, Electrochemical Interfaces in Energy Storage: Advances in Simulations, Methods and Models, CECAM Lausanne, Switzerland

3-7/07/24: *Probing Dynamics* at *Different Time Scales by Density Functional Theory*, ESPA2024 III Meeting of GEQC, Tarragona, Spain

23-26/05/23: *Multiscale modelling of liquids and electrolyte solutions under confinement*, Young Researchers' School on Theory and Simulation in Electrochemical Conversion Processes, École Normale Supérieure, Paris, France, CECAM-FR-MOSER

10/10/22: *CP2K: high performance electronic structure calculations*, Electronic Structure Software Development: Best Practices and Tools, CECAM, Lausanne, Switzerland, ESL22

05/09/22: *Advanced sampling for reactions at fluid/solid interfaces*, 20 Years of Metadynamics, CECAM, Lausanne, Switzerland, MTD22

29/08/22: *Connection between Water's Dynamical and Structural Properties: Insights from Ab Initio Simulations,* DFT 2022, Brussels, Belgium, DFT2022

13/06/22: *Osmotic transport at the aqueous 2D material interfaces from ab initio molecular dynamics simulations*, Atomistic simulations of interfacial processes in energy materials, Sorbonne University Pierre et Marie Campus Paris France, CECAM-FR-MOSER

16/05/22: *QM/MM approaches in ab initio molecular dynamics* in CP2K, Hybrid QMMM Approaches to biochemistry and beyond, CECAM, Lausanne, Switzerland, QMMM22

30/03/22: *Core level spectroscopy by real-time time-dependent DFT*, CONEXS Conference 2022, Newcastle University, UK CONEXS22

24/09/21: *Osmotic transport at the aqueous graphene and hBN interfaces from ab initio molecular dynamics simulations* , MolSimEng 20/21, Politecnico di Milano, Italy

2/09/21 : *Subsystem Density Functional Theory Augmented by a Delta Learning Approach to Achieve Kohn-Sham Accuracy*, Non-Covalent Interactions in Large Molecules and Extended Materials, CECAM-HQ-EPFL, Lausanne, Switzerland

20/05/21: *Water metal interfaces by ab initio molecular dynamics*, Physics and Chemistry of Electrified Interfaces, Thomas Young Centre, London, UK

09/12/19 : *Interfaces by ab initio molecular dynamics*, Operando Surface Science, 708. WE-Heraeus-Seminar, Bad Honnef, Germany

09/09/19 : *Molecules at the Electrochemical Interface: Understanding Experiments with Simulations*, Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM, Lausanne, Switzerland

27/08/19 : *Liquid solid interfaces by ab initio molecular dynamics*, Symposium on Catalysis, Delft, The Netherlands

22/07/19 : *Molecules at the Electrochemical interface: Understanding Experiments with Simulations*, CPMD Meeting 2019 Pushing the Boundaries of Molecular Dynamics, Lausanne, Switzerland

14/06/19 : *Molecules at the solid/liquid interface: understanding experiments with simulations*, CP2K users and developers symposium, London, UK

04/19 : *QM/MM approaches in ab initio molecular dynamics*, CECAM- Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and Beyond, CECAM, Lausanne, Switzerland

03/19 : *CP2K: GAPW & Electronic Properties*, Introduction to CP2K, Ghent, Belgium

08/18: *Gaussian augmented plane waves formalism for NEXAFS and NMR*, Workshop on Computational Spectroscopy, Padeborn University, Germany

06/18 : *Adsorbed molecules at the solid/liquid interface*, MolCH Meeting, Bern, Switzerland

02/18 : *Simulation of Processes @ quasi-2D Interfaces by ab initio MD*, Introduction to CP2K, Lyon, France

05/17: *QM/MM approaches in ab initio molecular dynamics*, CECAM- Hybrid QMMM Approaches to Biochemistry and Beyond, CECAM, Lausanne, Switzerland