Michele Ceriotti

Curriculum Vitae

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Institute of Materials, École Polytechnique Fédérale de Lausanne,
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Development and application of statistical sampling and machine-learning algorithms to achieve predictive atomic-scale modelling of molecules and materials, and to understand structure-property relations.

Current Post

Sep. 2020 –	**Associate Professor, Institute of Materials, EPFL** Principal Investigator, Laboratory of Computational Science and Modelling (COSMO)

Previous Posts

Nov. 2013 – Sep. 2020	EPFL, Assistant professor
Jan. 2011 – Oct. 2013	Junior Research Fellow, Merton College, University of Oxford (Prof. David Manolopoulos)
Jun. 2010 – Dec. 2010	Post-Doctoral Researcher, Swiss Federal Insititute of Technology, Zürich (Prof. Michele Parrinello)

Education

Jan. 2007 – May 2010	PhD in Physics, Swiss Federal Insititute of Technology, Zürich (Prof. Michele Parrinello)
Oct. 2004 – Oct. 2006	MSc in Materials Science, with honors, University of Milano - Bicocca (Prof. Marco Bernasconi)
Sep. 2001 – Oct. 2004	BSc in Materials Science, with honors, University of Milano - Bicocca

Prizes & Awards

2018	IUPAP–C10 Young Scientist Prize
2013	Volker Heine Young Investigator Award
2010	IBM Research Forschungspreis (http://www.c4.ethz.ch/ibmprize/index)
2010	ETH Medal for Ph.D. Thesis

Research and Grants

- More than 150 peer-reviewed articles, that have collected as of January 2023 more than 12000 citations. h-index: 59
- More than 200 invited talks, for conferences, workshops and departmental seminars
- Stong committment to open science, with several open-source projects (`http://ipi-code.org`, `http://gle4md.org`, `http://shiftml.org`, `http://alphaml.org`, `http://chemiscope.org`) and data dissemination activities
- More than 9M€ in competitive grants, including an ERC Starting Grant (2016) and an ERC Consolidator Grant (2021)

Service and Community Recognition

- Associate Editor for the Journal of Chemical Physics
- Member of the Editorial Board of Physical Review Materials
- Moderator of the physics.chem-ph section of the arXiv
- Spokeperson of the Psi-k Working Group on Statistical Sampling
- Organizer of a dozen workshops, schools and symposia
- Frequent reviews for journal articles and grant proposals
- Serving on several departmental and institutional committees at EPFL

Teaching and Mentoring

- Supervision of 20 PhD students (10 of which have already defended successfully)
- MSc course on “Statistical Mechanics”, Institute of Materials, EPFL (4 ECTS credits, 51 hours)
- BSc course on “Introduction to Atomic-Scale Modeling”, Institute of Materials, EPFL (2 ECTS credits, 39 hours)
- 28 hours course for Master and Ph.D. students at EPFL “Statistical methods in atomistic computer simulations”
- Coordination of an “advanced MOOC” on “Path Integral Methods”
- Invited lectures: Tokyo University (2020); TYC Masterclass, King’s College London (2016); PKU, Beijing (2013)

Selected Publications

A full list of publications, complete with up-to-date citation data, can be retrieved at https://scholar.google.com/citations?user=exWw7d0AAAAJ&hl=en.

1. J. Nigam, S. Pozdnyakov, G. Fraux, and M. Ceriotti. Unified Theory of Atom-Centered Representations and Message-Passing Machine-Learning Schemes. *J. Chem. Phys.* **156**.(20) (May 2022), 204115. DOI: 10.1063/5.0087042.
2. V. L. Deringer, N. Bernstein, G. Csányi, C. Ben Mahmoud, M. Ceriotti, M. Wilson, D. A. Drabold, and S. R. Elliott. Origins of Structural and Electronic Transitions in Disordered Silicon. *Nature* **589**.(7840) (Jan. 2021), 59–64. DOI: 10.1038/s41586-020-03072-z.
3. E. A. Engel, V. Kapil, and M. Ceriotti. Importance of Nuclear Quantum Effects for NMR Crystallography. *J. Phys. Chem. Lett.* **12**.(32) (Aug. 2021), 7701–7707. DOI: 10.1021/acs.jpclett.1c01987.
4. A. Grisafi, J. Nigam, and M. Ceriotti. Multi-Scale Approach for the Prediction of Atomic Scale Properties. *Chem. Sci.* **12**.(6) (2021), 2078–2090. DOI: 10.1039/D0SC04934D.
5. F. Musil, A. Grisafi, A. P. Bartók, C. Ortner, G. Csányi, and M. Ceriotti. Physics-Inspired Structural Representations for Molecules and Materials. *Chem. Rev.* **121**.(16) (Aug. 2021), 9759–9815. DOI: 10.1021/acs.chemrev.1c00021.
6. B. Cheng, G. Mazzola, C. J. Pickard, and M. Ceriotti. Evidence for Supercritical Behaviour of High-Pressure Liquid Hydrogen. *Nature* **585**.(7824) (Sept. 2020), 217–220. DOI: 10.1038/s41586-020-2677-y.
7. S. N. Pozdnyakov, M. J. Willatt, A. P. Bartók, C. Ortner, G. Csányi, and M. Ceriotti. Incompleteness of Atomic Structure Representations. *Phys. Rev. Lett.* **125** (2020), 166001. DOI: 10.1103/PhysRevLett.125.166001.
8. B. Cheng, E. A. Engel, J. Behler, C. Dellago, and M. Ceriotti. Ab Initio Thermodynamics of Liquid and Solid Water. *Proc. Natl. Acad. Sci. U. S. A.* **116**.(4) (Jan. 2019), 1110–1115. DOI: 10.1073/pnas.1815117116.
9. A. Grisafi, A. Fabrizio, B. Meyer, D. M. Wilkins, C. Corminboeuf, and M. Ceriotti. Transferable Machine-Learning Model of the Electron Density. *ACS Cent. Sci.* **5**.(1) (Jan. 2019), 57–64. DOI: 10.1021/acscentsci.8b00551.
10. D. M. Wilkins, A. Grisafi, Y. Yang, K. U. Lao, R. A. DiStasio, and M. Ceriotti. Accurate Molecular Polarizabilities with Coupled Cluster Theory and Machine Learning. *Proc. Natl. Acad. Sci. U. S. A.* **116**.(9) (Feb. 2019), 3401–3406. DOI: 10.1073/pnas.1816132116.
11. M. J. Willatt, F. Musil, and M. Ceriotti. Atom-Density Representations for Machine Learning. *J. Chem. Phys.* **150**.(15) (Apr. 2019), 154110. DOI: 10.1063/1.5090481.
12. A. Anelli, E. A. Engel, C. J. Pickard, and M. Ceriotti. Generalized Convex Hull Construction for Materials Discovery. *Phys. Rev. Mater.* **2**.(10) (Oct. 2018), 103804. DOI: 10.1103/PhysRevMaterials.2.103804.
13. B. Cheng, A. T. Paxton, and M. Ceriotti. Hydrogen Diffusion and Trapping in α -Iron: The Role of Quantum and Anharmonic Fluctuations. *Phys. Rev. Lett.* **120**.(22) (May 2018), 225901. DOI: 10.1103/PhysRevLett.120.225901.
14. A. Grisafi, D. M. Wilkins, G. Csányi, and M. Ceriotti. Symmetry-Adapted Machine Learning for Tensorial Properties of Atomistic Systems. *Phys. Rev. Lett.* **120**.(3) (Jan. 2018), 036002. DOI: 10.1103/PhysRevLett.120.036002.
15. T. E. Markland and M. Ceriotti. Nuclear Quantum Effects Enter the Mainstream. *Nat. Rev. Chem.* **2**.(3) (Feb. 2018), 0109. DOI: 10.1038/s41570-017-0109.
16. A. P. Bartók, S. De, C. Poelking, N. Bernstein, J. R. Kermode, G. Csányi, and M. Ceriotti. Machine Learning Unifies the Modeling of Materials and Molecules. *Sci. Adv.* **3**.(12) (Dec. 2017), e1701816. DOI: 10.1126/sciadv.1701816.
17. M. Ceriotti, W. Fang, P. G. Kusalik, R. H. McKenzie, A. Michaelides, M. A. Morales, and T. E. Markland. Nuclear Quantum Effects in Water and Aqueous Systems: Experiment, Theory, and Current Challenges. *Chem. Rev.* **116**.(13) (July 2016), 7529–7550. DOI: 10.1021/acs.chemrev.5b00674.
18. M. Rossi, P. Gasparotto, and M. Ceriotti. Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol. *Phys. Rev. Lett.* **117**.(11) (Sept. 2016), 115702. DOI: 10.1103/PhysRevLett.117.115702.
19. M. Ceriotti, J. Cuny, M. Parrinello, and D. E. Manolopoulos. Nuclear Quantum Effects and Hydrogen Bond Fluctuations in Water. *Proc. Natl. Acad. Sci. U. S. A.* **110**.(39) (Sept. 2013), 15591–15596. DOI: 10.1073/pnas.1308560110.
20. M. Ceriotti and D. E. Manolopoulos. Efficient First-Principles Calculation of the Quantum Kinetic Energy and Momentum Distribution of Nuclei. *Phys. Rev. Lett.* **109**.(10) (Sept. 2012), 100604. DOI: 10.1103/PhysRevLett.109.100604.
21. M. Ceriotti, G. A. Tribello, and M. Parrinello. Simplifying the Representation of Complex Free-Energy Landscapes Using Sketch-Map. *Proc. Natl. Acad. Sci. U. S. A.* **108**.(32) (Aug. 2011), 13023–13028. DOI: c.
22. M. Ceriotti, G. Bussi, and M. Parrinello. Langevin Equation with Colored Noise for Constant-Temperature Molecular Dynamics Simulations. *Phys. Rev. Lett.* **102**.(2) (Jan. 2009), 020601. DOI: 10.1103/PhysRevLett.102.020601.
23. M. Ceriotti, G. Bussi, and M. Parrinello. Nuclear Quantum Effects in Solids Using a Colored-Noise Thermostat. *Phys. Rev. Lett.* **103**.(3) (July 2009), 30603. DOI: 10.1103/PhysRevLett.103.030603.