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Stefano Martiniani

Academic Positions

Assistant Professor	**New York University** Dept. of Physics, Center for Soft Matter Research Dept. of Chemistry, Simons Center for Computational Physical Chemistry Courant Institute of Mathematical Sciences	2022 – present
Assistant Professor	**University of Minnesota - Twin Cities** Dept. of Chemical Engineering and Materials Science	2019 – 2021

Education

BSc Chemistry with First Class Honors	**Imperial College London**	2012
MPhil Scientific Computing with Distinction	**University of Cambridge**	2013
PhD Chemistry (Outstanding Thesis Award)	**University of Cambridge**	2017
Postdoctoral – Physics	**New York University**	2017 – 2019

Academic summary

Publications	18 research articles (8 lead author, 9 corresp. author).
Media	Research highlighted on PRL cover, PCCP cover, Nature, Nature Materials, Physics, Physics Today (1), Physics Today (2), New Scientist, Science & Vie, Sky News, ANSA.
Presentations	40 past talks (25 invited), 8 upcoming invited talks, 9 posters.
Teaching Innovation	Developed graduate course "Physics of Neural Systems" at NYU, and U. Minnesota's first ML course outside the CS/Stats departments, CHEN 5802 "Machine Learning for Chemical Sciences and Engineering".
Funding	NSF III 2132995 (PI), NSF CESER 2039575 (Co-PI), NIH R01 GM146372 (Co-I).
Leadership	Co-PI and Machine Learning Technical Lead of ColabFit project. Co-founder and member of organizing committee for KIMReview journal.
Mentorship	Currently leading a group of 6 graduate students, 3 postdocs and 2 staff scientists. **Past trainees:** 1 PhD student in ChEn, 9 undergraduate (3 published), 1 master, 1 high-school students (1 published).

Awards

Simons Foundation Faculty Fellowship	New York University	2022 – 2025
Outstanding Thesis Prize	Dept. of Chemistry, University of Cambridge	2017
Gates Cambridge Scholarship	University of Cambridge	2013 – 2017
Benefactors Scholarship	St. John's College, University of Cambridge	2013 – 2017

Prize for Best Physical Chemistry Research Project (BS/MS Thesis)	Dept. of Chemistry, Imperial College London	2012
Undergraduate Research Fellowship	Dept. of Chemistry, Imperial College London	2012

Funding

1. **Role:** PI; **Title:** "EAGER: Quantifying the error landscape of deep neural networks"*;* **Program:** NSF III; **Funds:** $149,225 ; **Duration:** 2 years (Oct 2021 - Sept 2023); **Award number:** 2132995.
2. **Role:** co-PI; **Title:** "Data CI Pilot: CI-Based Collaborative Development of Data-Driven Interatomic Potentials for Predictive Molecular Simulations"*;* **Program:** NSF CESER, DMR; **Funds:** $1,127,993; **Duration:** 2 years (Oct 2020 - Sept 2022); **Award number:** 2039575.
3. **Role:** co-I; **Title:** "Engineering Protein Developability"; **Program:** NIH GM R01; **Funds:** $1,815,456; **Duration:** 4 years (Oct 2022-2026); **Award number**: GM146372.

Publications (*trainee, †contributed equally)

Preprints

18. A. W. Golinski*, Z. D. Schmitz*, G. H. Nielsen, B. Johnson*, D. Saha*, S. Appiah*, B. J. Hackel, **S. Martiniani**, "Predicting and Interpreting Protein Developability via Transfer of Convolutional Sequence Representation", *bioRxiv preprint* 2022.11.21.517400

Peer-reviewed articles

17. M. Kasiulis*, **S. Martiniani**, "When you can't count sample! Computable entropies beyond equilibrium from basin volumes", *Papers in Physics, 15, 150001 (2023).*
    - Invited perspective in "Focus Series on Challenges in Granular Matter", Editors: K. Daniels, L. Pugnaloni, J. Zhao.
16. C. Anzivino, M. Casiulis*, T. Zhang,* A. S. Moussa, **S. Martiniani**, A. Zaccone, "Estimating random close packing in polydisperse and bidisperse hard spheres via an equilibrium model of crowding", *J. Chem. Phys., 158, 044901 (2023)*
15. S. Ro, B. Guo, A. Shih*, T.V. Phan, R.H. Austin, D. Levine, P.M. Chaikin, **S. Martiniani**, "Model-Free Measurement of Local Entropy Production and Extractable Work in Active Matter", *Phys. Rev. Lett.* 129, 220601 (2022).
    - **Cover article** for *Phys. Rev. Lett.*
    - Highlighted as **Editor's Suggestion** in *Phys. Rev. Lett.*
    - Highlighted in **"Measuring Entropy in Active-Matter Systems"**, *Physics* 15, 179 (2022)
14. A. W. Golinski*, K. M. Mischler, S. Laxminarayan, N. Neurock, M. Fossing, H. Pichman, **S. Martiniani**, B. J. Hackel, "High-Throughput Developability Assays Enable Library-Scale Identification of Producible Protein Scaffold Variants", *Proc. Natl. Acad. Sci.***,** 118, 23 (2021)

13. A. Cavagna, P. M. Chaikin, D. Levine, **S. Martiniani**, A. Puglisi, M. Viale, "Vicsek Model by Time-Interlaced Compression: a Dynamical Computable Information Density", *Phys. Rev. E* 103, 062141 (2021)

12. **S. Martiniani**, Y. Lemberg, P. M. Chaikin, D. Levine, "Correlation lengths in the language of computable information", *Phys. Rev. Lett.*, 125, 170601 (2020)

11. **S. Martiniani**, P. M. Chaikin, D. Levine, "Quantifying hidden order out of equilibrium", *Phys. Rev. X,* 9, 011031 (2019)
    - Highlighted in "**File compression uncovers hidden order**", *Physics Today* (2019).

10. **S. Martiniani**, K. J. Schrenk, K. Ramola, B. Chakraborty, D. Frenkel, "Numerical test of the Edwards conjecture shows that all packings become equally probable at jamming", *Nature Physics*, 13, 848–851 (2017)
    - Highlighted in "**Intuition harnessed in the name of particle packing**", *Nature*, 546, 575 (2017).
    - Highlighted in "**A thermodynamic theory of granular materials endures**", *Physics Today* 70, 9 (2017).
    - Highlighted in "**Material Witness: A jammy guess?**", *Nature Materials*, 15**,** 1227 (2016).

9. D. Frenkel, K. J. Schrenk, **S. Martiniani** "Monte Carlo sampling for stochastic weight functions", *Proc. Natl. Acad. Sci.,* 114, 27 (2017)

8. A. J. Ballard, R. Das, **S. Martiniani**, D. Mehta, L. Sagun, J. D. Stevenson, D. J. Wales, "Energy Landscapes for Machine Learning", *Phys. Chem. Chem. Phys.,* 19**,** 12585 (2017)
    - **Cover article** for *Phys. Chem. Chem. Phys.*

7. **S. Martiniani**, K. J. Schrenk, J. D. Stevenson, D. J. Wales, D. Frenkel, "Structural analysis of high dimensional basins of attraction", *Phys. Rev. E* 94, 031301 (2016)

6. **S. Martiniani**, K. J. Schrenk, J. D. Stevenson, D. J. Wales, D. Frenkel, "Turning intractable counting into sampling: computing the configurational entropy of three-dimensional jammed packings", *Phys. Rev. E* 93, 012906 (2016)

5. A. J. Ballard, **S. Martiniani**, J. D. Stevenson, S. Somani, D. J. Wales, "Exploiting the potential energy landscape to sample free energy", *WIREs Comput. Mol. Sci.* 5, 273 (2015)

4. **S. Martiniani**, J. D. Stevenson, D. J. Wales, D. Frenkel, "Superposition Enhanced Nested Sampling", *Phys. Rev. X* 4, 031034 (2014)

3. C. Magistris†, **S. Martiniani†**, N. Barbero, J. Park, C. Benzi, A. Anderson, C. H. Law, C. Barolo, B. C. O'Regan, "Near-infrared absorbing squaraine dye with extended π conjugation for dye-sensitized solar cells", *Renewable Energy* 60, 672 (2013)

2. C. E. Richards, A. Y. Anderson, **S. Martiniani**, C. Law, B. C. O'Regan, "The Mechanism of Iodine Reduction by TiO2 Electrons and the Kinetics of Recombination in Dye-Sensitized Solar Cells", *J. Phys. Chem. Lett.* **3**, 1980 (2012)

1. **S. Martiniani**, A. Y. Anderson, C. Law, B. C. O'Regan and C. Barolo, "New insight into the regeneration kinetics of dye sensitised solar cells", *Chem. Commun.* 48, 2406 (2012)

Peer-reviewed conference abstracts

1. R. Rawat*, D. Heeger, **S. Martiniani**, "Coherence influences the dimensionality of communication subspaces". Cosyne Abstracts (2023).

Ph.D. thesis

S. Martiniani, "On the complexity of energy landscapes: algorithms and a direct test of the Edwards conjecture", University of Cambridge (2017)
- Awarded "Outstanding Thesis Prize", Dept. of Chemistry, University of Cambridge

Conference presentations and seminars

Talks (*invited)

Upcoming

1. * Workshop on Geometric Constraints: Materials, Graphs and Matroids, Rigidity and Packings, Fields Institute for Research in Mathematical Sciences, Jul 2023
2. * Courant Institute, Applied Maths Seminar, May 2023
3. * Complex Systems Seminar, Northwestern University, May 2023
4. * Symposium: Systems for Fitting, Uncertainty Quantification, Selection and Use of Interatomic Models, Mach Conference, April 2023
5. * CMU (Arpa-E) Scientific Machine Learning Webinar Series, March 2023
6. * Levich Institute Seminar, CUNY, March 2023
7. * Focus session: "Information theory and Physics", APS March meeting 2023
8. * Short Course "Computational modeling and information theory: from grains to bits", APS March meeting 2023

Past

1. * Computations in Science Seminar**,** Dept. of Physics, University of Chicago, Jan 2022
   Title: *"The other side of entropy"*
2. * 123rd Statistical Mechanics Conference, Rutgers University, Dec 2022
   Title: "*Play. Pause. Rewind. Model Free Measurement of Local Entropy Production and Extractable Work in Active Matter.*"
3. * Colloquium, Center for Computational Mathematics, Flatiron Institute, Dec 2022
   Title: *"The other side of entropy"*
4. * Research Seminar, Santa Fe Institute, Nov 2022
   Title: *"The other side of entropy"*
5. * Research Seminar, Center for Nonlinear Studies, Los Alamos National Laboratory, Nov 2022
   Title: "*Play. Pause. Rewind. Model Free Measurement of Local Entropy Production and Extractable Work in Active Matter.*"
6. * Research Seminar (remote), Dept. of Chemistry, UT Austin, Host: Devarajan Thirumalai, Oct 2022
   Title: *"The other side of entropy"*

7. Frontiers in Computational Chemistry: The NYU Simons Center Inaugural Symposium, Oct 2022
   Title: "*Play. Pause. Rewind. Model Free Measurement of Local Entropy Production and Extractable Work in Active Matter.*"
8. * Theoretical Chemistry Seminar, Dept. of Chemistry, University of Cambridge, Aug 2022
   Title: *"The Other Side of Entropy"*
9. Physics of Information workshop, Dept. of Physics, New York University, May 2022
   Title: *"The Other Side of Entropy"*
10. * Research Seminar (remote), Condensed Matter Theory group, Dept. of Physics, University of Oxford, Host: Shivaji Sondhi, Apr 2022
    Title: *"The other Side of entropy"*
11. APS March meeting, Session D20: Active Matter in Complex Environments II, Chicago, Mar 2022
    Title: *"Play. Pause. Rewind. Measuring local entropy production and extractable work in active matter"*
12. AIChE Annual Meeting, Session: Active Colloidal Systems, Boston, Nov 2021
    Title: *"Play. Pause. Rewind. Measuring local entropy production and extractable work in active matter"*
13. APS March Meeting (remote), Session Y06: Memory Formation in Matter: Encoding, Reading, and Design II, Mar 2021
    Title: *"Squeezing order out of disorder"*
14. * Research Seminar, Dept. of Chemistry, New York University, Mar 2021
    Title: *"The other side of entropy"*
15. * Machine Learning Seminar, University of Minnesota - Twin Cities, Dec 2020
    Title: "*Design and Discovery in the Protein Fitness Landscape"*
16. Applied Physics "Socioloquium" (remote), SEAS, Harvard University, Main speaker: P.M. Chaikin, Contributors: **S. Martiniani**, D. Frenkel, Host: Eric Mazur, Jun 2020
    Title: *"Information and Order"*
17. * Seminar, Chemical Theory Center, Dept. of Chemistry, University of Minnesota - Twin Cities, May 2020
    Title: *"Are some packings more equal than others? A direct test of the Edwards conjecture."*
18. * APS March Meeting, Denver (CO), Session J31: Workshop: Grand Challenges in Soft Matter and Opportunities for Microgravity Research, Mar 2020 (meeting cancelled for COVID-19 crisis)
    Title: *"Squeezing order out of disorder"*
19. * Geomechanics Seminar, Dept. of Civil, Environmental and Geo- Engineering, University of Minnesota - Twin Cities, Feb 2020
    Title: *"Are some packings more equal than others? A direct test of the Edwards conjecture"*
20. * Condensed Matter Seminar, Dept. of Physics, University of Minnesota - Twin Cities, Dec 2019
    Title: *"Squeezing order out of disorder"*
21. * Solid Mechanics Research Seminar, Dept. of Aerospace Engineering and Mechanics, University of Minnesota - Twin Cities, Nov 2019
    Title: *"Are some packings more equal than others? A direct test of the Edwards conjecture"*
22. 17th Annual Northeastern Granular Materials Workshop, New York University, Jun 2018
    Title: *"Taking the numerical calculations of granular entropy forward"*

23. APS March Meeting, Boston, Mar 2019
    Title: *"Characterizing elusive correlation lengths by computable information density"*
24. * Research Seminar, Centre for Theoretical Biological Physics, Rice University, Feb 2019
    Title: *"Quantifying hidden order out of equilibrium"*
25. * Research Seminar, Dept. of Chemical Engineering and Material Science, University of Minnesota - Twin Cities, Feb 2019
    Title: *"Quantifying hidden order out of equilibrium"*
26. * Research Seminar, Dept. of Chemistry, University of Illinois Urbana-Champaign, Jan 2019
    Title: *"Quantifying hidden order out of equilibrium"*
27. * Research Seminar, Santa Fe Institute, Jan 2019
    Title: *"Quantifying hidden order out of equilibrium"*
28. * Research Seminar, Dept. of Chemistry, University of Colorado Boulder, Dec 2018
    Title: *"Quantifying hidden order out of equilibrium"*
29. MRSEC Seminar, New York University, Oct 2018
    Title: *"Quantifying hidden order out of equilibrium"*
30. 16th Annual Northeastern Granular Materials Workshop, Yale University, Jun 2018
    Title: *"Quantifying hidden order out of equilibrium"*
31. * DAMPT Statistical Physics and Soft Matter Seminar, University of Cambridge, May 2018
    Title: *"Quantifying hidden order out of equilibrium"*
32. * Mach Conference, Annapolis (MD), Apr 2018
    Title: *"Taking the numerical calculation of granular entropy forward: a new look at the yielding transition"* - **session keynote**
33. * Army Research Lab (ARL), Aberdeen Proving Ground (MD), Apr 2018
    Title: *"Quantifying hidden order out of equilibrium"*
34. APS March Meeting, Los Angeles (CA), Mar 2018
    Title: *"Quantifying hidden order out of equilibrium"*
35. Edwards Centre for Soft Matter Inaugural Meeting, University of Cambridge, Jan 2017
    Title: *"Are some packings more equal than others? A direct test of the Edwards conjecture"*
36. Recent Advances on the Glass and Jamming Transition, CECAM Workshop, Lausanne, Switzerland, Jan 2017 - **poster prize talk**
    Title: *"Are some packings more equal than others? A direct test of the Edwards conjecture"*
37. * 3rd International Conference on Packing Problems, Shanghai, China, Sept 2016
    Title: *"Turning intractable counting into sampling: Computing the configurational entropy of three-dimensional jammed packings"*
38. StatPhys 26, Lyon, France, Jul 2016
    Title: *"Turning intractable counting into sampling: Computing the configurational entropy of three-dimensional jammed packings"*
39. * Institute for Multiscale Simulations, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany, Aug 2015
    Title: *Turning intractable counting into sampling: the mean basin volume method"*

40. Gordon Conference on Granular and Granular-Fluid Flow, Stonehill College, Easton (MA), Jul 2014
    Title: *"Numerical Calculation of Granular Entropy"*

Posters

1. GRC Neurobiology of Cognition: Neural Circuits Supporting Cognitive Function, Newry (ME), Jul 2022
   Title: *"Towards a unifying and analytically tractable framework for neural dynamics"*
2. IEEE European School of Information Theory, Bertinoro, Italy, May 2018
   Title: *"Quantifying hidden order out of equilibrium"*
3. Recent Advances on the Glass and Jamming Transition, CECAM Workshop, Lausanne, Switzerland, Jan 2017
   Title: *"Are some packings more equal than others? A direct test of the Edwards conjecture"*
4. Soft Matter – Theoretical and Industrial Challenges, University of Cambridge, UK, Sept 2016
   Title: *"Are some packings more equal than others? A direct test of the Edwards conjecture"*
5. International Workshop on Jamming and Granular Matter, Queen Mary University of London, UK, Jul 2016
   Title: *"Turning intractable counting into sampling: Computing the configurational entropy of three-dimensional jammed packings"*
6. Machine Learning Summer School, Kyoto, Japan, Aug 2015
   Title: *"Computing extremely high-dimensional volumes"*
7. Italian Soft Days, Università la Sapienza, Rome, Italy, Sept 2014
   Title: *"Numerical Calculation of Granular Entropy"*
8. Advanced School in Soft Condensed Matter 'Solutions in the Spring', Homerton College, Cambridge, UK, Apr 2014
   Title: *"Superposition Enhanced Nested Sampling"*
9. International Soft Matter Conference, Università la Sapienza, Rome, Italy, Sept 2013
   Title: *"Superposition Enhanced Nested Sampling"*

Organized workshops and conference sessions

1. Workshop: "*Physics of Information*", Dept. of Physics, New York University, May 2022
2. Focus Session: *"Machine Learning for Biomolecular Design and Simulation"*, APS March Meeting 2021

Extended stays

1. Aspen Center for Physics, "Learning Dynamical Models from Biophysical Data", Jun 2022

Teaching

2019-present

PHYS-GA 2061 "Physics of Neural Systems" (Spring 2023)

CHEM-UA 652 "Thermodynamics & Kinetics" (Fall 2022)

CHEN 3201 "Numerical Methods for Chemical Engineering" (Spring 2020, co-instructor; Spring 2021, Fall 2021 lead instructor)

	CHEN 8754 "Quantitative Analysis, Design and Synthesis of Biotechnological Systems." Delivered 2.5h of content on "Information theory for biochemical signal pathways" (Spring 2021, contributing lecturer)
	CHEN 5595 "Data Driven Discovery for the Chemical Sciences" (Fall 2020)
	MATS 3001 "Thermodynamics of Materials" (Fall 2019, co-instructor)
	Workshop on Machine Learning for Chemical Engineering and Materials Science ($\sim$ 40 participants, year-long).
2013 - 2015	**Mathematics tutor** for natural sciences and computer science students in the Tripos IA (first year) at Magdalene College, Cambridge. Tutorials consisted of year-long 1 hour weekly meetings with 3 or 4 groups of 2 students each.
2013	**Laboratory demonstrator** for Tripos IA (first year) organic chemistry practicals (University of Cambridge).

Mentorship (*current trainee)

2019-present

Postdoc	*Mathias Casiulis, *Guanming Zhang, *Amit Gupta
PhD	**Physics:** *Praharsh Suryadevara. **Chemistry:** *Asit Pal. **Mathematics:** *Aaron Shih, *Shivang Rawat, *Satyam Anand. **Chemical Engineering:** Alexander Golinski (co-advised, NSF GRFP), *Zach Schmidtz (co-advised).
Research staff	*Gregory Wolfe, *Eric Fuemeler.
Master	**Mathematics:** Zayyam Mohammed.
Undergraduate	**Physics:** Bryce Johnson. **Mathematics:** Kyrie Xie. **Chemical Engineering:** Diya Saha, Sandya Appiah, Daniel Ribeiro, Jiwon Kim (Honors Thesis), Remi Bougie (Honors Thesis). **Materials Science**: Vijay Vallurupalli. **Statistics:** Kovic Odhiambo.
High-school	Tom Zhang (Westport, CT).

2014-2019

U. Cambridge	**Day-to-day supervisor** for 2 Physics Part III final year project (one awarded Part III prize for best computational physics project); 1 exchange master student (awarded distinction from TU-Munich).

Service

Peer-review	PRL, PRX, PRE, PNAS, Nat. Neuroscience, J. Chem. Phys., J. Stat. Phys, J. Comp. Phys.

Review panels	NSF Molecular Foundations for Biotechnology	2022
Other	Gates Cambridge Junior Treasurer, University of Cambridge Responsible for planning and managing a £60k budget.	2016 – 2017

Synergistic activities

Outreach

1. NYU Proud to Be First Advocate and Proud to Be First Mentor;
2. Host for high-school students seeking research experience (Summer 2022);
3. Jury member for "Science Court", an interdisciplinary course in the University of Minnesota Honors Program designed to combat polarization in American society and strengthen democracy (Fall 2020);
4. Primary School PS-154 STEM Professionals Day, Brooklyn, NY (2019).

Open Science

Co-PI and Machine Learning technical lead of Colabfit project. Advancing software infrastructure for Findable, Accessible, Interoperable and Reusable (FAIR) implementations of machine learning potentials, and for archiving, discovering, and accessing datasets.

Dissemination

1. My research has been broadly highlighted by scientific and news media worldwide, including in Nature, Nature Materials, Physics, Physics Today (1), Physics Today (2), New Scientist, Science & Vie, Sky News, ANSA.
2. Co-founder and member of organizing committee of KIMReview, a journal publishing commentaries on important articles related to classical molecular simulations of hard and soft matter materials (launched Aug 2022).

Other professional experience

Cadet (active duty)	Italian Army, "Scuola Military Teulié", Milan	2005 – 2008