Address: Department of Physics,
New York University,
726 Broadway, New York, NY, 10013
e-mail: sm7683@nyu.edu
web: martinianilab.org

Stefano Martiniani

Academic Positions

Assistant Professor — **New York University** — 2022 – present
Dept. of Physics, Center for Soft Matter Research
Dept. of Chemistry, Simons Center for Computational Physical Chemistry
Courant Institute of Mathematical Sciences
Center for Data Science (Affiliated)

Assistant Professor — **University of Minnesota - Twin Cities** — 2019 – 2021
Dept. of Chemical Engineering and Materials Science
Dept. of Physics (Graduate faculty)
Data Science (Graduate faculty)

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 — 22 research articles (8 lead author, 13 corresponding author), 1 commentary, 2 peer-reviewed conference abstracts (COSYNE).

Media — Research highlighted on PRL cover, PCCP cover, Nature, Nature Materials, Physics (1), Physics (2), Physics Today (1), Physics Today (2), New Scientist, Science & Vie, Sky News, ANSA.

Presentations — 51 past talks (35 invited), 9 posters.

Funding — NSF OAC 2311632 (PI), NIH R01 EY035242 (PI), NSF III 2132995 (PI), NSF CESER 2039575 (Co-PI), NIH R01 GM146372 (Co-I).
Total PI/co-PI extramural funding: $7,857,022 ($6,729,029 as PI).

Leadership — Lead PI of FERMat project, involving 8 investigators across 4 universities (NYU, UMN, UF, BYU) and 1 industry partner (Amazon Web Services);
Machine Learning Lead/co-PI of ColabFit project;
Co-founder and member of organizing committee for KIMReview journal.

Teaching Innovation — Developed graduate course "Physics of Neural Systems" at NYU, and UMN's first non-CS/Stats ML course "Machine Learning for Chemical Sciences and Engineering".

Mentorship — Currently leading a group of 7 graduate students, 3 postdocs, 2 research scientists, 1 research assistant. **Past trainees:** 1 PhD student in ChEn, 1

master, 12 undergraduates (3 published), 4 high-school students (1 published), 3 ColabFit interns (2 published).

Awards

Gallery of Soft Matter Prize	APS Division of Soft Matter	2024
CZI Pairs Pilot Project Award	Chan Zuckerberg Initiative	2024
Interdisciplinary Early Career Scientist Prize	Int. Union of Pure and Applied Physics	2023
Simons Foundation Faculty Fellowship	New York University	2022 – 2025
Outstanding Thesis Prize	Dept. of Chemistry, U. of Cambridge	2017
Gates Cambridge Scholarship	University of Cambridge	2013 – 2017
Benefactors Scholarship	St. John's College, U. of Cambridge	2013 – 2017
Prize for Best Physical Chemistry Research Project (BS/MS Thesis)	Dept. of Chemistry, Imperial College	2012
Undergraduate Research Fellowship	Dept. of Chemistry, Imperial College	2012

Funding

1. **Role:** PI; **PD/PI:** Martiniani; **Title:** "Theme 2: AI Institute for Extreme Computing Materials (AI-XCoM)"; **Program:** NYU Mega Grants Initiative Seed Fund; **Funds:** $25,000; Duration: 11 months (Feb 2024 - Dec 2024);
2. **Role:** PI**; PD/PI:** Martiniani (contact), Fenton; **Title:** "Machine Learning the Biomolecular Basis of Memory Persistence"; **Program:** CZI Pairs Pilot Project Awards; **Funds:** $200,000; Duration: 2 years (March 2024 - March 2025); **Award number:** 2024-338565.
3. **Role:** PI; **PD/PI:** Martiniani**; Title:** "GOALI: Frameworks: At-Scale Heterogeneous Data based Adaptive Development Platform for Machine-Learning Models for Material and Chemical Discovery"; **Program:** NSF OAC; **Funds:** $4,500,000; Duration: 5 years (Oct 2023 - Sept 2028); **Award number:** 2311632.
4. **Role:** PI; **PD/PI:** Heeger (contact), Martiniani; **Title:** "Recurrent circuit model of neural response dynamics in V1"; **Program:** NIH NEI R01 (multi-PI); **Funds:** $1,879,804; **Duration:** 4 years (Sept 2023 - Sept 2027); **Award number:** EY035242.
5. **Role:** PI; **PD/PI:** Martiniani; **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.
6. **Role:** co-PI; **PD/PI:** Tadmor; **Title:** "Data CI Pilot: CI-Based Collaborative Development of Data-Driven Interatomic Potentials for Predictive Molecular Simulations"*;* **Program:** NSF CESER; **Funds:** $1,127,993; **Duration:** 2 years (Oct 2020 - Sept 2022); **Award number:** 2039575.
7. **Role:** co-I; **PD/PI:** Hackel; **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

23. T.V. Phan, S. Li, D. Ferreris, R. Morris, J. Bos, B. Guo, **S. Martiniani**, P. Chaikin, Y.G. Kevrekidis, R.H. Austin, "Social Physics of Bacteria: Avoidance of an Information Black Hole", *arXiv preprint* arXiv:2401.16691 (2024)

22. S Anand*, X Ma, S Guo, **S. Martiniani**, X. Cheng, "Bacteria Through Obstacles: Unifying Fluxes, Entropy Production, and Extractable Work in Living Active Matter", *arXiv preprint* arXiv:2308.08421 (2023)

21. S. Rawat*, **S. Martiniani**, "Explicit rational function solutions for the power spectral density of stochastic linear time-invariant systems", a*rXiv preprint* arxiv:2305.19890 (2023)

20. A. Shih*, M. Casiulis*, **S. Martiniani**, "Fast Generation of Spectrally-Shaped Disorder", a*rXiv preprint* arXiv:2305.15693 (2023)
    - Awarded Gallery of Soft Matter Prize and highlighted in *Physics,* 17, 41 (2024).

Peer-reviewed articles

19. J. A. Vita*, E. G. Fuemmeler*, A. Gupta*, G.P. Wolfe*, A. Q. Tao*, R. S. Elliott, **S. Martiniani**, E. B. Tadmor, "ColabFit Exchange: open-access datasets for data-driven interatomic potentials", J. Chem. Phys. 159, 154802 (2023)

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", ACS Synth. Biol. 12, 9, 2600 (2023)

17. M. Casiulis*, **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

2. R. Rawat*, D. Heeger, **S. Martiniani**, "A comprehensive large-scale model of primary visual cortex (V1)". Cosyne Abstracts (2024).

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

Commentaries

1. **S. Martiniani**, "Bit-propelled Active Matter". Journal Club for Condensed Matter Physics (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

Data, models, and software products

ML models

1. A. Gupta, E.B. Tadmor, **S. Martiniani**, Parallel NequIP Equivariant GNN for Si developed by Gupta et al. (2024) v000. OpenKIM; 2024. doi:10.25950/d7a965ba

Software (maintained)

1. **KLIFF v1.0** github.com/openkim/kliff/tree/v1 (2024 - present)
   Framework for training physics-based and ML-based interatomic potentials implemented in PyTorch and deployed through popular simulators such as LAMMPS via OpenKIM.

2. **KUSP** github.com/ipcamit/kusp (2024 - present)
   The KIM Utility for serving potential provides an easy and quick way to deploy any potential, ML or otherwise to the KIM API.

3. **Spectre** https://github.com/martiniani-lab/spectre (2023 - present)
   Implementation of element-wise and recursive solutions for the power spectral density of biological stochastic dynamical systems at fixed points introduced by Rawat and Martiniani.

4. **FReSCo** github.com/martiniani-lab/FReSCo (2023 - present)
   Command Line interface for ColabFit Exchange.

5. **Colabfit Data Lake** github.com/colabfit/data-lake (2023 - present)
   Platform to request inclusion of an existing dataset or to submit a new dataset to the ColabFit Exchange.

6. **ColabFit CLI** github.com/colabfit/colabfit-cli (2023 - present)
   Command Line interface for ColabFit Exchange.

7. **ColabFit Exchange** colabfit.org (2022 - present)
   Curated repository of first principles datasets for training data-driven interatomic potentials based on machine learning. With 450+ datasets, the ColabFit Exchange is the largest and most diverse public database of first principle data for machine learning interatomic potentials.

8. **ColabFit Tools** colabfit.github.io/colabfit-tools (2022 - present)
   Tools for constructing and manipulating datasets for fitting interatomic potentials in/from the Colabfit Exchange.
9. **Libdescriptor** github.com/colabfit/data-lake (2022 - present)
   High performance library for representations of atomic environments.
10. **Sweetsourcod** github.com/martiniani-lab/sweetsourcod (2017 - present)
    This library is a collection of methods to estimate the entropy of sequences by data compression (source coding).
11. **PyCG_DESCENT** github.com/martiniani-lab/PyCG_DESCENT (2014 - present)
    Python wrapper for the Hager and Zang CG_DESCENT algorithm. CG_DESCENT is a conjugate gradient algorithm for solving an unconstrained minimization problem.
12. **mcpele** github.com/martiniani-lab/mcpele (2014 - present)
    Flexible and efficient Monte Carlo general purpose framework and MPI/mpi4py based Replica Exchange Method. Seamlessly integrated with pele.
13. **pele** github.com/martiniani-lab/pele (2014 - present)
    Tools for global optimization, attractor finding and energy landscape exploration.

Talks (*invited)

Upcoming

1. * Mach conference, Workshop: Systematic Discovery of Materials Across Composition and Structure, Annapolis (MD), Apr 2024
2. * Flash talk, NYU AI Research Symposium "Bridging AI Innovation and Societal Impact", New York, April 2024
3. * CZI 2024 Neuroscience Kickoff Series, Circuitry & Plasticity, Webinar, April 2024
4. * Condensed Matter Seminar, Dept. of Physics, UMass Amherst, May 2024
5. * Physical Chemistry Seminar, UC Irvine, May 2024
6. * ACS Fall Meeting, Symposium: Elevating Biomolecular Simulations With Data-Driven Approaches", August 2024

Past

1. * Minisymposium on "Suppression and Variability in Visual Cortex", Society for Neuroscience annual meeting, Washington D.C., Nov 2023
   Title: *"ORGaNICs: A Recurrent Circuit Theory of Normalization"*
2. * Colloquium, Center for Computational Neuroscience, Flatiron Institute, Nov 2023
   Title: "*Recurrent Circuit Theory of Cortical Communication"*
3. * Machine Learning Potentials - StAtus and FuturE (MLP-SAFE), Virtual Workshop, Jul 2023
   Title: *"ColabFit: An Integrated Platform for Designing, Training, Sharing, and Deploying Machine Learning Interatomic Potentials at Scale."*

4. * Conclave on Complexity in Physical Interacting Systems, Computation, and Thermodynamics, Los Alamos National Laboratory, Santa Fe (NM), Jul 2023
   Title: "*Play. Pause. Rewind.Linking local entropy production, fluxes, and extractable work in active matter.*"
5. Energy Landscapes Workshop (Long talk, 1h), Porquerolles (France), Jun 2023
   Title: *"From Slices to Volumes: Unveiling the Geometry of High-Dimensional Energy Landscapes.*"
6. * Complex Systems Seminar, Dept. of Physics, Northwestern University, May 2023
   Title: *"Cortical circuit theory of interareal communication"*
7. * Symposium: Systems for Fitting, Uncertainty Quantification, Selection and Use of Interatomic Models, Mach Conference, April 2023
   Title: *"Colabfit: An integrated Platform for Designing, Training, Sharing, and Deploying Machine Learning Interatomic Potentials at Scale"*
8. * Webinar, Scientific Machine Learning Webinar Series, CMU Arpa-E, March 2023
   Title: *"Colabfit: An integrated Platform for Designing, Training, Sharing, and Deploying Machine Learning Interatomic Potentials at Scale"*
9. * Levich Institute Seminar, CUNY, March 2023
   Title: *"The other side of entropy"*
10. * Invited talk, Focus session: "Information theory and Physics", APS March meeting 2023
    Title: *"The other side of entropy"*
11. * Invited tutorial, Short Course "Computational modeling and information theory: from grains to bits", APS March meeting 2023
    Title: *"The other side of entropy"*
12. * Computations in Science Seminar**,** Dept. of Physics, University of Chicago, Jan 2023
    Title: *"The other side of entropy"*
13. * 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.*"
14. * Colloquium, Center for Computational Mathematics, Flatiron Institute, Dec 2022
    Title: *"The other side of entropy"*
15. * Research Seminar, Santa Fe Institute, Nov 2022
    Title: *"The other side of entropy"*
16. * 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.*"
17. * Research Seminar (remote), Dept. of Chemistry, UT Austin, Host: Devarajan Thirumalai, Oct 2022
    Title: *"The other side of entropy"*
18. 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.*"

19. * Theoretical Chemistry Seminar, Dept. of Chemistry, University of Cambridge, Aug 2022
    Title: *"The Other Side of Entropy"*
20. Physics of Information workshop, Dept. of Physics, New York University, May 2022
    Title: *"The Other Side of Entropy"*
21. * Research Seminar (remote), Condensed Matter Theory group, Dept. of Physics, University of Oxford, Host: Shivaji Sondhi, Apr 2022
    Title: *"The other Side of entropy"*
22. 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"*
23. AIChE Annual Meeting, Session: Active Colloidal Systems, Boston, Nov 2021
    Title: *"Play. Pause. Rewind. Measuring local entropy production and extractable work in active matter"*
24. APS March Meeting (remote), Session Y06: Memory Formation in Matter: Encoding, Reading, and Design II, Mar 2021
    Title: *"Squeezing order out of disorder"*
25. * Research Seminar, Dept. of Chemistry, New York University, Mar 2021
    Title: *"The other side of entropy"*
26. * Machine Learning Seminar, University of Minnesota - Twin Cities, Dec 2020
    Title: "*Design and Discovery in the Protein Fitness Landscape"*
27. 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"*
28. * 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."*
29. * 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"*
30. * 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"*
31. * Condensed Matter Seminar, Dept. of Physics, University of Minnesota - Twin Cities, Dec 2019
    Title: *"Squeezing order out of disorder"*
32. * 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"*
33. 17th Annual Northeastern Granular Materials Workshop, New York University, Jun 2018
    Title: *"Taking the numerical calculations of granular entropy forward"*
34. APS March Meeting, Boston, Mar 2019
    Title: *"Characterizing elusive correlation lengths by computable information density"*

35. * Research Seminar, Centre for Theoretical Biological Physics, Rice University, Feb 2019
    Title: *"Quantifying hidden order out of equilibrium"*
36. * Research Seminar, Dept. of Chemical Engineering and Material Science, University of Minnesota - Twin Cities, Feb 2019
    Title: *"Quantifying hidden order out of equilibrium"*
37. * Research Seminar, Dept. of Chemistry, University of Illinois Urbana-Champaign, Jan 2019
    Title: *"Quantifying hidden order out of equilibrium"*
38. * Research Seminar, Santa Fe Institute, Jan 2019
    Title: *"Quantifying hidden order out of equilibrium"*
39. * Research Seminar, Dept. of Chemistry, University of Colorado Boulder, Dec 2018
    Title: *"Quantifying hidden order out of equilibrium"*
40. MRSEC Seminar, New York University, Oct 2018
    Title: *"Quantifying hidden order out of equilibrium"*
41. 16th Annual Northeastern Granular Materials Workshop, Yale University, Jun 2018
    Title: *"Quantifying hidden order out of equilibrium"*
42. * DAMPT Statistical Physics and Soft Matter Seminar, University of Cambridge, May 2018
    Title: *"Quantifying hidden order out of equilibrium"*
43. * Mach Conference, Annapolis (MD), Apr 2018
    Title: *"Taking the numerical calculation of granular entropy forward: a new look at the yielding transition"* - **session keynote**
44. * Army Research Lab (ARL), Aberdeen Proving Ground (MD), Apr 2018
    Title: *"Quantifying hidden order out of equilibrium"*
45. APS March Meeting, Los Angeles (CA), Mar 2018
    Title: *"Quantifying hidden order out of equilibrium"*
46. 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"*
47. 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"*
48. * 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"*
49. StatPhys 26, Lyon, France, Jul 2016
    Title: *"Turning intractable counting into sampling: Computing the configurational entropy of three-dimensional jammed packings"*
50. * Institute for Multiscale Simulations, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany, Aug 2015
    Title: *Turning intractable counting into sampling: the mean basin volume method"*
51. 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. Working group: "Theory and circuits of cortical function and corticocortical communication", Aspen Center for Physics, Jul 2023.
2. Workshop: "*Physics of Information*", Dept. of Physics, New York University, May 2022
3. Focus Session: *"Machine Learning for Biomolecular Design and Simulation"*, APS March Meeting 2021

Extended stays

1. Aspen Center for Physics, "Theory and circuits of cortical function and corticocortical communication", Jul 2023
2. Aspen Center for Physics, "Learning Dynamical Models from Biophysical Data", Jun 2022

Teaching

2019-present	**PHYS-UA 2061** "Mathematical Physics" (Spring 2024)
	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).

University Service

NYU FAS	Member, Computational Science Initiative Committee	2023
NYU Physics	Member, Graduate Admission Committee	2024
	Member, Grant Administrator Search Committee	2024
	Member, CSMR Faculty Search Committee	2022
NYU Chemistry	Member, Simons Center Core Team	2023 - 2024
	Member, Colloquium Committee	2022 - 2024
	Member, Theory Faculty Search Committee	2023
	Member, Graduate Admission Committee	2022 - 2023
	Member, Simons Center Administrator Search Committee	2022

External Service

Conferences	Reviewer for COSYNE 2024	
Journals	Co-founder and member of organizing committee of KIMReview	2023 - present
	Reviewer for PRL, PRX, PRE, PNAS, Nat. Neuroscience, J. Chem. Phys., J. Stat. Phys, J. Comp. Phys.	2016 - present
Review panels	NSF Molecular Foundations for Biotechnology	2022
Other	Gates Cambridge Junior Treasurer, University of Cambridge	2016 – 2017

Synergistic activities

Outreach	1. Member of Public School 3 STEAM (A for Art) committee, New York, NY (2023 - present)
	2. Member of organizing committee for Conferences for Undergraduate Women in Physics (CUWiP) 2025, hosted by NYU (2023 - present).

3. NYU Proud to Be First Advocate and Proud to Be First Mentor;

4. Host for high-school students seeking research experience (2022, 2023);

5. 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 (2020);

6. Public School 154 STEM Professionals Day, Brooklyn, NY (2019).

Dissemination

1. Video entry to APS-DSOFT Gallery 2024 - awarded jury prize.

2. Video entry to APS-DSOFT Gallery 2022.

Open Science

1. Lead PI of FERMat project, developing Machine Learning "foundation" models for materials and molecular discovery, and associated cyber-infrastructure.

2. Machine Learning Lead/co-PI of Colabfit project, providing the largest public database of first principle data for training ML Interatomic Potentials.

Media

1. Research highlighted by scientific and news media worldwide, including in Nature, Nature Materials, Physics (1), Physics (2), Physics Today (1), Physics Today (2), New Scientist, Science & Vie, Sky News, ANSA.

2. Press-release by U.S. Senate Majority Leader Chuck Schumer and U.S. Senator Kirsten Gillibrand announcing the FERMat project.

Interviews

1. Main guest on the program "Si può fare" by Radio24 (radio station of the Italian financial newspaper of record "Il Sole 24 Ore", 2.2M listeners per day) to talk about Artificial Intelligence and foundation models for materials discovery. The interview is available from minute 20 of this podcast.

Current and past group members

Graduate Students

Alexander Golinski — Ph.D. Chemical Engineering, 2021, University of Minnesota, co-advised with Ben Hackel (primary). **Thesis:** Data-driven approach to engineering protein evolvability and developability. **Awards:** NSF GRFP.

Zach Schmitz — Current Chemical Engineering Ph.D. student at University of Minnesota, co-advised with Ben Hackel (primary), anticipated graduation 2024.

Shivang Rawat — Current Mathematics Ph.D. student, anticipated graduation 2024. Transferred from University of Minnesota.

Aaron Shih — Current Mathematics Ph.D. student, anticipated graduation 2024. Transferred from University of Minnesota.

Praharsh Suryadevara — Current Physics Ph.D. student, anticipated graduation 2024. Transferred from University of Minnesota.

Satyam Anand — Current Mathematics Ph.D. student, anticipated graduation 2025. Transferred from University of Minnesota.

Asit Pal	Current Chemistry Ph.D. student, anticipated graduation 2026.
Tom Egg	Current Chemistry Ph.D. student, anticipated graduation 2028.
Ben Johnston	Current Physics Ph.D. student, anticipated graduation 2028.

Postdocs

Mathias Casiulis	Postdoctoral Associate, Dept. of Physics, NYU, 2022 - present
Guanming Zhang	Postdoctoral Associate, Dept. of Physics, NYU, 2023 - present
Philipp Hoellmer	Simons Center Fellow, Dept. of Chemistry, NYU, 2024 - present

Research Scientists

Eric Fuemmeler	Research Scientist, Dept. of Aerospace Engineering & Mechanics, UMN, 2021 - present (co-advised with Ellad Tadmor)
Amit Gupta	Research Scientist, Dept. of Aerospace Engineering & Mechanics, UMN, 2021 - present (co-advised with Ellad Tadmor)

Research Assistants

Gregory Wolfe	Research Assistant, Dept. of Physics, NYU, 2023 - present

Undergraduate and Master students

Master	**Mathematics:** Zayyam Mohammed.
Undergraduate	**Physics:** Bryce Johnson. **Mathematics:** Kyrie Xie, Carmel Pe'er, Orion Runjia Yang, Charlie Chen. **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), Juhee Park (Fort Lee High School, NJ), Gabriel Magnasco-Farinas (HSAS-Lehman, NY), Milan Lustig (Cold Spring Harbor High School, NY).

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).

Other professional experience

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