

Alexander Hampel

Associate Data Scientist
CCQ, Flatiron Institute
Simons Foundation

+1 917-306-6334

mail@alexander-hampel.de

the-hampel

alexander-hampel.de

/in/the-hampel

Languages

- German: native speaker
- English: full professional proficiency
- Latin: elementary proficiency

Personal interests

- technology & programming
- running & cycling
- tennis
- audio
- news

References

- Prof. Antoine Georges
ageorges@flatironinstitute.org
Collège de France / Flatiron Institute
- Prof. Cyrus Dreyer
cyrus.dreyer@stonybrook.edu
Stonybrook University
- Prof. Andrew J. Millis
amillis@flatironinstitute.org
Columbia University /
Flatiron Institute
- Prof. Claude Ederer
claudio.ederer@mat.ethz.ch
Materials Theory, ETH Zürich

Work experience

- 2022 - present **Associate Data Scientist** CCQ, Flatiron Institute
software development for the TRIQS open source software project
under supervision of Oliver Parcollet, oparcollet@flatironinstitute.org
- 2019 - 2022 **Flatiron Research Fellow** CCQ, Flatiron Institute
PostDoc researcher under supervision of Prof. Antoine Georges
- 2016 - 2019 **Research group IT support** Materials Theory, ETH Zürich
- responsible for Linux workstations and local servers of group
 - development and maintenance of group gitlab repositories
 - coordinating acquisition of new hardware and software

Education

- 2015 - 2019 **PhD, Materials Science** Materials Theory, ETH Zürich
supervisor: Claude Ederer, claudio.ederer@mat.ethz.ch
Interplay between structural, electronic, and magnetic properties in rare-earth nickelates
- 2013 - 2015 **MSc, Physics** Universität Hamburg, Germany
Master thesis: *Interplay of Spin-Orbit Coupling and Electron Correlations in Iridate Compounds*
supervisor: Frank Lechermann, flecherm@physnet.uni-hamburg.de
- 2009 - 2013 **BSc, Computing in Science: Physics** Universität Hamburg, Germany
Bachelor thesis: *Oxygen Vacancies in Ceria Surfaces*
supervisor: Frank Lechermann, flecherm@physnet.uni-hamburg.de

Technical skills

- programming: **Python, C++**, cmake, Bash, MPI, Fortran, ML basics
- data analysis & processing with the scientific python stack, i.e. numpy, scipy, jupyter, pandas, matplotlib, plotly, dash (see github.com/TRIQS/FermiSee)
- electronic structure codes: TRIQS, VASP, Quantum Espresso, Wannier90
- profound knowledge in architecture and use of HPC systems
- continuous integration techniques: Docker, github CI, Jenkins, unit tests

Organization

- 2023 **Co-organizer of the TRIQS summer school 2023**
organization and lecturer at the first TRIQS school in Paris
- 2020 - present **Co-organizer of the DMFT / Quantum Embedding Meeting at CCQ**
organization of the biweekly seminar series with international speakers.
- 2020 - present **Deployment of electronic structure codes for HPC system**
Provide users of the HPC facilities at the Flatiron Institute a scripted module environment to build common electronic structure codes:
github.com/flatironinstitute/ccq-software-build

Publications - selection

Google scholar profile: scholar.google.com/citations?user=lghTPb0AAAAJ&hl

- "Stabilizing the calculation of the self-energy in dynamical mean-field theory using constrained residual minimization" *arXiv* (2023) H. LaBollita, J. Kaye, and A. Hampel
- "Correlation-Induced Octahedral Rotations in SrMoO₃" *Phys. Rev. B* **104** (2021) A. Hampel, J. Lee-Hand, A. Georges, and C. E. Dreyer
- "Quantum embedding methods for correlated excited states of point defects: Case studies and challenges" *Phys. Rev. B* **105** (2022) L. Muechler, D. I. Badrtdinov, A. Hampel, J. Cano, M. Rösner, C. E. Dreyer
- "solid_dmft: gray-boxing DFT+ DMFT materials simulations with TRIQS" *Journal of Open Source Software* **7** (2022) M. E. Merkel, A. Carta, S. Beck, and A. Hampel

Teaching

- supervising intern PhD student at Flatiron Institute: "Automatic tail fitting for noisy QMC self-energies in Dynamical Mean Field Theory", Harrison LaBollita
- supervision of summer intern under graduate student: "FermiSee: WebApp for electronic structure visualization and phenomenology", Shonel Rahim
- tutor for the "International summer school on computational quantum materials 2022", Sherbrooke, Canada
- tutor for the "Wannier 2022 Summer School", Trieste, Italy
- supervising intern PhD student at Flatiron Institute: "Interplay between breathing-mode distortions and magnetic order in rare-earth nickelates from ab initio magnetic models", Danis I. Badrtdinov *Phys. Rev. B* **104**, 054403 (2021)
- mentoring a master student project: Tobias Esswein
- mentoring a bachelor thesis: "Analysis of structural distortions in CaFeO₃ using first-principles calculations": Alexander Gillmann
- tutor for the two Practica: *Statistical Analysis* and *Computer Simulation of Materials*, Materials Department, ETH Zürich
- teaching Assistant for the Course: *Simulation Techniques in Materials Science*, Materials Department, ETH Zürich

Attended conferences and schools (selection)

Invited talks

09/2023	TRIQS developer and user meeting 2023	Paris, France
05/2023	Wannier90 Developer meeting	Daresbury, UK
08/2022	33rd IUPAP Conference on Computational Physics	Austin, USA
06/2022	TRIQS developer and user meeting 2022	Paris, France
02/2022	Condensed matter seminar talk at Stony Brook University	USA
01/2022	Invited seminar talk University of Geneva	Switzerland
09/2019	Invited seminar talk at the ITP	University of Bremen, Germany
06/2019	TRIQS developer and user meeting 2019	Paris, France
12/2017	MARVEL Junior Seminar	Lausanne, Switzerland

Contributed talks

03/2022	American Physical Science Conference	Chicago, USA
03/2021	American Physical Science Conference	virtual, USA

Schools & Workshops

06/2023	Nvidia workshop: Fundamentals of Deep Learning	New York, USA
06/2018	Workshop: Exploiting Supercomputers and Containers for Data Science	Zurich, Switzerland
02/2017	ViCoM Winter School on Computational Magnetism	Vienna, Austria
05/2016	International Summer School on Computational Methods for Quantum Materials	Sherbrooke, Canada

List of Publications

Alexander Hampel

October 27, 2023

Google scholar profile: scholar.google.com/citations?user=lgHTPb0AAAAJ&hl

2023

- **Stabilizing the calculation of the self-energy in dynamical mean-field theory using constrained residual minimization**
H. LaBollita, J. Kaye, and A. Hampel
arXiv (2023), arxiv.org/abs/2309.01407
- **TRIQS/Nevanlinna: Implementation of the Nevanlinna Analytic Continuation method for noise-free data**
I. Sergei, A. Hampel, N. Wentzell, and E. Gull
arXiv (2023), arxiv.org/abs/2310.01266
- **Dielectric Environment Sensitivity of Carbon Centers in Hexagonal Boron Nitride**
D. I. Badrtdinov, C. Rodriguez-Fernandez, M. Grzeszczyk, Z. Qiu, K. Vaklinova, P. Huang, A. Hampel, K. Watanabe, T. Taniguchi, L. Jiong, M. Potemski, C. E. Dreyer, M. Koperski, M. Rösner
Small Journal **2300144** (2023), doi.org/10.1002/sml.202300144
- **Low-rank Green's function representations applied to dynamical mean-field theory**
N. Sheng, A. Hampel, S. Beck, O. Parcollet, N. Wentzell, J. Kaye, and K. Chen
Phys. Rev. B **107** (2023), doi.org/10.1103/PhysRevB.107.245123
- **Conductivity of infinite-layer NdNiO₂ as a probe of spectator bands**
H. LaBollita, A. Hampel, J. Karp, A. S. Botana, and A. J. Millis
Phys. Rev. B **107** (2023), doi.org/10.1103/PhysRevB.107.205155
- **Orbital polarization, charge transfer, and fluorescence in reduced-valence nickelates**
M. R. Norman, A. S. Botana, J. Karp, A. Hampel, H. LaBollita, A. J. Millis, G. Fabbris, Y. Shen, M. P. M. Dean
Phys. Rev. B **107** (2023), doi.org/10.1103/PhysRevB.107.165124

2022

- **solid_dmft: gray-boxing DFT+ DMFT materials simulations with TRIQS**
M. E. Merkel, A. Carta, S. Beck, and A. Hampel
Journal of Open Source Software **7(77)**, 4623 (2022), doi.org/10.21105/joss.04623
- **Ab-initio investigation of Er³⁺ defects in tungsten disulfide**
G. I. López-Morales, A. Hampel, Gustavo E. López, Vinod M. Menon, J. Flick, and C. A. Meriles
Computational Materials Science **210** (2022), doi.org/10.1016/j.commatsci.2021.111041
- **Quantum embedding methods for correlated excited states of point defects: Case studies and challenges**

L. Muechler, D. I. Badrtdinov, A. Hampel, J. Cano, M. Rösner, C. E. Dreyer
Phys. Rev. B **105**, 235104 (2022), doi.org/10.1103/PhysRevB.105.235104

- **Electronic structure of the highly conductive perovskite oxide SrMoO₃**
E. Cappelli, A. Hampel, A. Chikina, E. Bonini Guedes, G. Gatti, A. Hunter, J. Issing, N. Biskup, M. Varela, C. E. Dreyer, A. Tamai, A. Georges, F. Y. Bruno, M. Radovic, and F. Baumberger
Phys. Rev. Materials **6**, 075002 (2022), doi.org/10.1103/PhysRevMaterials.6.075002
- The effects of strain in multi-orbital superconductors: the case of Sr₂RuO₄
S. Beck, A. Hampel, M. Zingl, C. Timm, and A. Ramires
Phys. Rev. Research **4**, 023060 (2022), doi.org/10.1103/PhysRevResearch.4.023060
- Charge self-consistent electronic structure calculations with dynamical mean-field theory using Quantum ESPRESSO, Wannier90 and TRIQS
S. Beck, A. Hampel, O. Parcollet, C. Ederer, and A. Georges
Journal of Physics: Condensed Matter **34**, 235601 (2022), doi.org/10.1088/1361-648X/ac5d1c
- Dynamical Mean Field Studies of Infinite Layer Nickelates: Physics Results and Methodological Implications
H. Chen, A. Hampel, J. Karp, F. Lechermann, and A. J. Millis
Frontiers in Physics **10**, 835942 (2022)
- Superconductivity and Antiferromagnetism in NdNiO₂ and CaCuO₂ : A Cluster DMFT Study
J. Karp, A. Hampel, and A. J. Millis
Phys. Rev. B **105**, 205131 (2022), doi.org/10.1103/PhysRevB.105.205131

2021

- Sensing strain-induced symmetry breaking by reflectance anisotropy spectroscopy
M. Volpi, S. Beck, A. Hampel, H. Galinski, A. Sologubenko and R. Spolenak
Applied Physics Letters **119**, 151602 (2021), doi.org/10.1063/5.0060930
- Investigation of photon emitters in Ce-implanted hexagonal boron nitride
G. I. López-Morales, M. Li, A. Hampel, S. Satapathy, N. V. Proscia, H. Jayakumar, A., D. Pagliero, G. E. Lopez, V. M. Menon, J. Flick, and C. A. Meriles
Opt. Mater. Express **11**, 3478-3485 (2021), doi.org/10.1364/OME.434083
- First-principles study of the electronic, magnetic, and crystal structure of perovskite molybdates
J. Lee-Hand, A. Hampel, and C. E. Dreyer
Phys. Rev. Materials **5**, 8 (2021), doi.org/10.1103/PhysRevMaterials.5.085001
- Interplay between breathing-mode distortions and magnetic order in rare-earth nickelates from ab initio magnetic models
D. I. Badrtdinov, A. Hampel, and C. E. Dreyer
Phys. Rev. B **104**, 054403 (2021), doi.org/10.1103/PhysRevB.104.054403
- **Correlation-Induced Octahedral Rotations in SrMoO₃**
A. Hampel, J. Lee-Hand, A. Georges, and C. E. Dreyer
Phys. Rev. B **104**, 035102 (2021), doi.org/10.1103/PhysRevB.104.035102
- Dependence of DFT+DMFT Results on the Construction of the Correlated Orbitals
J. Karp, A. Hampel, and A. J. Millis
Phys. Rev. B **103**, 195101 (2021), doi.org/10.1103/PhysRevB.103.195101

- Wave functions, electronic localization, and bonding properties for correlated materials beyond the Kohn-Sham formalism
A. D. N. James, E. I. Harris-Lee, A. Hampel, M. Aichhorn, and S. B. Dugdale
Phys. Rev. B **103**, 035106 (2021), doi.org/10.1103/PhysRevB.103.035106

2020

- Comparative Many-Body Study of $\text{Pr}_4\text{Ni}_3\text{O}_8$ and NdNiO_2
J. Karp, A. Hampel, M. Zingl, Antia S. Botana, H. Park, M. R. Norman, and A. J. Millis
Phys. Rev. B **102**, 245130 (2020), doi.org/10.1103/PhysRevB.102.245130
- Effect of charge self-consistency in DFT+DMFT calculations for complex transition metal oxides
A. Hampel, S. Beck, and C. Ederer
Phys. Rev. Research **2**, 033088 (2020), doi.org/10.1103/PhysRevResearch.2.033088

2019

- Interplay between structural, electronic, and magnetic properties in rare-earth nickelates
A. Hampel
PhD Thesis (2019), doi.org/10.3929/ethz-b-000372219
- Mechanism and Control Parameters of the Metal-Insulator Transition in Nickelates
O. E. Peil, A. Hampel, C. Ederer, and A. Georges
Phys. Rev. B **99**, 245127 (2019), doi.org/10.1103/PhysRevB.99.245127
- Energetics of the coupled electronic-structural transition in the rare-earth nickelate
A. Hampel, P. Liu, C. Franchini, and C. Ederer
npj Quantum Materials **4**, 5 (2019), doi.org/10.1038/s41535-019-0145-4

2017

- Interplay between breathing mode distortion and magnetic order in rare-earth nickelates $R\text{NiO}_3$ within DFT+ U
A. Hampel and C. Ederer
Phys. Rev. B **96**, 165130 (2017), doi.org/10.1103/PhysRevB.96.165130

2015

- Low-energy model and electron-hole doping asymmetry of single-layer Ruddlesden-Popper iridates
A. Hampel, C. Piefke, and F. Lechermann
Phys. Rev. B **92**, 085141 (2015), doi.org/10.1103/PhysRevB.92.085141