Dr. Johannes Margraf

Group Leader

Fritz-Haber-Institut der Max-Planck-Gesellschaft
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Academic Positions

Fritz-Haber-Institute / Research Group Leader
FEBRUARY 2021 - PRESENT, BERLIN

Chemical machine learning and electronic structure theory.

Technical University Munich / PostDoc and Group Leader
APRIL 2017 - JANUARY 2021, MUNICH

Machine learning in chemical reaction space.

University of Florida / PostDoc
MARCH 2016 -MARCH 2017, GAINESVILLE

Linking many-body and single-particle methods in quantum chemistry.

Education

PhD / FAU Erlangen-Nürnberg

Physical and Computational Chemistry (2015)

M.Sc. / FAU Erlangen-Nürnberg

Molecular Nanoscience (2012)

B.Sc. / FAU Erlangen-Nürnberg

Molecular Science (2012)

Postdoctoral and Thesis Advisors

Timothy Clark, University of Erlangen

Rodney J. Bartlett, University of Florida

Karsten Reuter, FHI Berlin

Research Supervision

Currently directly supervising 8 PhD students and 3 PostDocs.
Supervised >10 undergraduate Theses (B.Sc. and M.Sc.).

Funding and Fellowships

Mentoring of self-funded PostDocs and PhD Students
2017-2022
Funding for PostDocs via the Alexander-von-Humboldt Foundation (1) and PhD students via the China Scholarship Council (2) and Fonds der Chemischen Industrie (1).

IGGSE Project Grant / International Graduate School for Science and Engineering
2017
Funding for a collaborative project with two PhD students (3 years) in chemistry and computer science.

Postdoctoral Fellowship / TUM University Foundation
2018
Personal Grant

Return Fellowship / Alexander-von-Humboldt-Foundation
2017
Personal Grant

Feodor-Lynen-Fellowship / Alexander-von-Humboldt-Foundation
2016
Personal Grant

Beilstein PhD Scholarship / Beilstein Foundation
2012-2015
Personal Grant

Leadership Roles

Co-Organization of Psi-k Workshops *Modern Approaches to Coupling Scales In Materials Simulations* in 2018 and 2020.

Academic editor for the open-access journal *PeerJ Physical Chemistry* since 2019.

Conference Presentations

12 invited talks and department seminars (e.g. at Cambridge, Korean Advanced Institute of Science and Technology, University of Luxembourg), 9 contributed talks at international conferences and workshops (e.g. at Symposium Theoretische Chemie, ACS Meetings, Sanibel Symposium, DPG Meetings).

Teaching Experience

Teaching and co-developing M.Sc. level courses on *Solid State Theory* and *Advanced Electronic Structure Theory* at TU Munich. Currently developing a M.Sc. level course on *Chemical Machine Learning* at Uni Potsdam. Teaching B.Sc. level courses on *Introductory Quantum Mechanics* and *Scientific Programming* at TU Munich.

Recent Representative Publications

(Total: 61, h-Index: 26 (Google Scholar))

(1) Staacke, C.; Wengert, S.; Kunkel, C.; Csányi, G.; Reuter; K; **Margraf, J. T.**
Kernel Charge Equilibration: Efficient and Accurate Prediction of Molecular Dipole Moments with a Machine-Learning Enhanced Electron Density Model.
Machine Learning: Science and Technology **2022**, *in press*.

(2) **Margraf, J. T.**; Ulissi, Z.; Jung, Y.; Reuter, K.
Heterogeneous Catalysis in Grammar School.
Journal of Physical Chemistry C **2022**, *126*, *2931−2936*.

(3) Keller, E.; Tsatsoulis, T.; Reuter, K.; **Margraf, J. T.**
Regularized Second-Order Correlation Methods for Extended Systems.
Journal of Chemical Physics **2022**, *156*, 024106.

(4) Wengert, S.; Csányi, G.; Reuter, K.; **Margraf, J. T.**
Data-Efficient Machine Learning for Molecular Crystal Structure Prediction.
Chemical Science **2021**, *12*, 4536−4546.

(5) **Margraf, J. T.**; Reuter, K.
Pure Non-Local Machine-Learned Density Functional Theory for Electron Correlation.
Nature Communications **2021**, *12*, 344.

(6) Kunkel, C.; **Margraf, J. T.**; Chen, K.; Oberhofer, H.; Reuter, K.
Active Discovery of Organic Semiconductors.
Nature Communications **2021**, *12*, 2422.

(7) Stocker, S.; Csányi, G.; Reuter, K.; **Margraf, J. T.**
Machine Learning in Chemical Reaction Space.
Nature Communications **2020**, *11*, 5505.

(8) **Margraf, J. T.**; Kunkel, C.; Reuter, K.
Towards Density Functional Approximations from Coupled Cluster Correlation Energy Densities.
Journal of Chemical Physics **2019**, *150*, 244116.

(9) **Margraf, J. T.**; Bartlett, R. J.
Coupled Cluster and Many-Body Perturbation Theory for Fractional Charges and Spins.
Journal of Chemical Physics **2018**, *148*, 221103.

(10) **Margraf, J. T.**; Reuter, K.
Making the Coupled Cluster Correlation Energy Machine-Learnable.
Journal of Physical Chemistry A **2018**, *122*, 6343.