TACO Newsletter

03/2023

Content

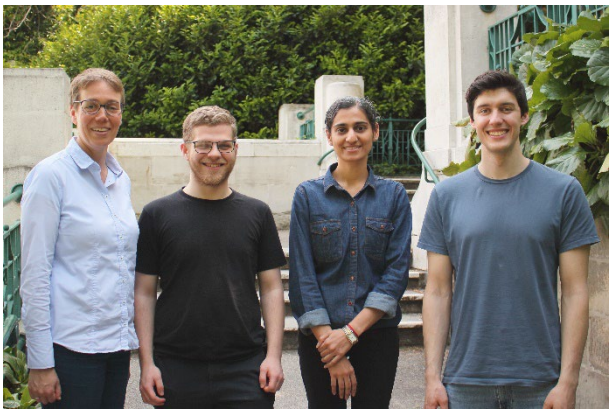
Reporting period: April – May 2023

1. Personnel Developments

Subproject P11 (Ellen Backus) has new personnel: In March, Lukas Bogner started as a master's student. Welcome to TACO!

Furthermore, Harsharan Kaur strengthens P11 as a new postdoc as of May 1. Welcome to TACO!

Group P11 has thus grown significantly:



Carolin Faller finished her master's degree and continues as a Ph.D. student in subproject P03 led by Georg Kresse. Congratulations, Carolin!

Andreas Grüneis' ERC-funded project "Chemical Accuracy for Complex Oxides" was assumed as an affiliated project to TACO. His Ph.D. students Sita Schönbauer and Thomas Plaikner will soon start to work on the project. Details about the project can be found on our website, and you can listen to a short video with Andreas on our YouTube channel.

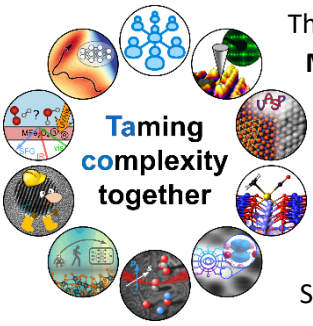
Are there personnel developments in your TACO subproject? Tell the science manager Stefan Uttenthaler about it!

2. Upcoming Events

Upcoming TACO talks in June:

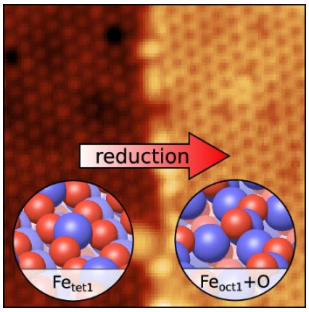
Date	Speaker	*Title*
June 13	Roland Netz (FU Berlin)	*Ions and water at aqueous interfaces* (joint TACO-IAP seminar)
June 19	Thomas Pock (TU Graz)	*Total Variation for Image Processing* (TA[CO]lloquium)
June 26	Angelika Kühnle (U. Bielefeld)	*Mineral-water interfaces investigated at the molecular level* (TA[CO]lloquium)

Individual invitations for the talks will follow.

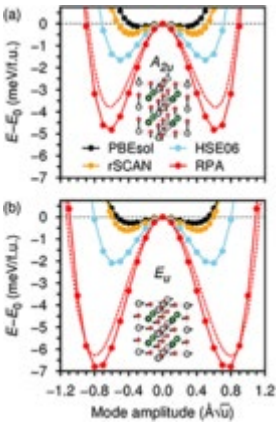


The highlight of the year will be our conference **"TAming COmplexity in Materials (TACO): Synergies between Experiment and Modeling"**, which will take place at TUtheSky from September 24-27. Mark your calendars! Confirmed invited speakers are: Bilge Yildiz (MIT), Boris Kozinsky (Harvard University), Beatriz Roldan (FHI Berlin), Karsten Reuter (FHI Berlin), Martin Setvin (Charles University Prague), Ralf Drautz (Ruhr University Bochum), Tanja Cuk (University of Colorado, Boulder), Johannes Kästner (University of Stuttgart), and Zdeñek Dohnalek (PNNL). Registration for the conference will open soon.

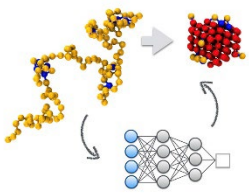
3. TACO Papers



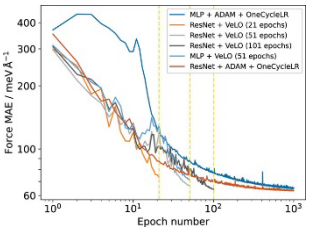
Several TACO papers were published in the reporting period. A total of three (!) TACO subprojects, namely P02 (Diebold), P04 (Parkinson), and P07 (Franchini), joined forces for the article titled "Oxygen-Terminated (1×1) Reconstruction of Reduced Magnetite Fe3O4(111)" by Florian Kraushofer et al., published in *The Journal of Physical Chemistry Letters*. Well done!



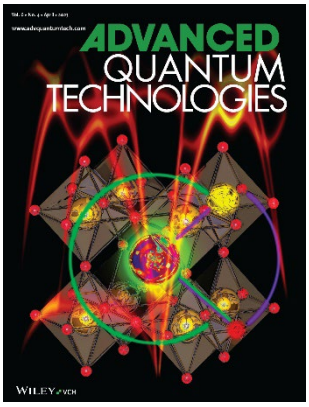
Carla Verdi et al. published the article titled "Quantum paraelectricity and structural phase transitions in strontium titanate beyond density functional theory" in *Physical Review Materials*. It is a joint paper of two TACO subprojects: P03 (Kresse) and P07 (Franchini).



Hendrik Jung et al., with the participation of Christoph Dellago (P12), presented a new machine-guided path sampling algorithm that learns the mechanisms of molecular self-organization. The paper was published in *Nature Computational Science*, and the Faculty of Physics of the University of Vienna published a news item about it on their website.



Another paper comes out of the Madsen group (P09): "Deep ensembles vs. committees for uncertainty estimation in neural-network force fields: Comparison and application to active learning", published by Jesus Carrete et al. in *The Journal of Chemical Physics*.



The article "Temperature-Dependent Anharmonic Phonons in Quantum Paraelectric $KTaO_3$ by First Principles and Machine-Learned Force Fields" by Ranalli et al., announced already in the previous TACO Newsletter edition, made an appearance on the cover page of *Advanced Quantum Technology* – congratulations!

Do you have a new TACO publication? Inform the science manager Stefan Uttenthaler about your outstanding scientific work!

4. New Projects and Grants

No newly approved grants were reported.

5. Awards and Achievements

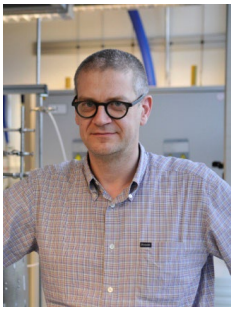
Michael Schmid, Co-PI in P02, was awarded the ICSOS Surface Structure Prize 2023 for his outstanding achievements in the development and application of methods to elucidate the surface structures of metal alloys, surface oxides, bulk oxides, and single-atom catalysts using scanning probe microscopies and complementary DFT and quantitative LEED methods. TU Wien announced a news item on this occasion. Congratulations, Michael!

Carla Verdi, Co-PI in P03, secured a permanent lecturer position down under at the University of Queensland. Congratulations, Carla!

6. Miscellaneous

We have a couple of new videos on our YouTube channel. Michail Stamatakis talked about "Unravelling Complexity in Heterogeneous Catalysis via High Fidelity Kinetic Monte Carlo Simulation" at the TA[CO]lloquium on March 20.

On April 17, we enjoyed Kristian Sommer Thygesen's colloquium presentation about "Data-Driven Materials Design".



Christophe Coperet gave a joint TACO-IAP seminar about "Surface Organometallic Chemistry for Controlled Functionalization and Molecular Understanding of Surfaces: Supported Single-Site Catalysts and Beyond". The (non-public) video is available on our YouTube channel for rewatching.

Andreas Grüneis presents his newly affiliated ERC project in a short video.

Our YouTube channel is an excellent opportunity to follow inspiring talks even when you missed them or listen to them again. You are welcome to subscribe to the channel and give the videos some thumbs-up!

If you are on Twitter, you can follow our account here; if you are on LinkedIn, you will find the same opportunity here.