Group picture of the TACO PhD Meeting 2026 at Gasthof Flackl in Reichenau an der Rax.

TACO Newsletter

No. 03, June 2026

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Reporting period: April – May 2026

1. Personnel Developments

Bianca Anghinelli is a new master's student in Karin Föttinger's subproject P10. You might have met her at the TACO PhD Meeting in April, in which she participated. Welcome to TACO!

Nico Unglert successfully defended his PhD thesis on March 19. He was hitherto a PhD student associated with Georg Madsen's subproject P09. His thesis title is "*Prediction of phase diagrams using machine-learning-backed nested sampling*". In the picture, you can see Nico with his external examiners, Christoph Dellago and Reinhard Maurer, as well as his supervisor, Georg Madsen. For the time being, Nico continues as a postdoc in Georg's group while waiting for the decisions about fellowship proposals. Congratulations, Dr Nico, and fingers crossed!

Harsharan Kaur, who was a postdoc in Ellen Backus' subproject P11, has left TACO and now works as a postdoc at TU Dresden in the „Physics of Life" group of Ellen Adams. We wish her the best of success for her future endeavours!

Please inform the TACO science manager, Stefan Uttenthaler, about personnel developments in your subproject.

2. Upcoming Events

The **TACO Retreat** will take place at the Steinschalerhof in Rabenstein an der Pielach from **September 28 to 30, 2026**. The invited keynote speakers will be: **Gustav Bihlmayer**, **Stefan Blügel** (both Forschungszentrum Jülich), **Claudia Draxl** (HU Berlin), **David Duncan** (University of Nottingham), **Veronique Van Speybroeck** (University of Ghent), and **Bert Weckhuysen** (Utrecht University). We can look forward to many interesting talks!

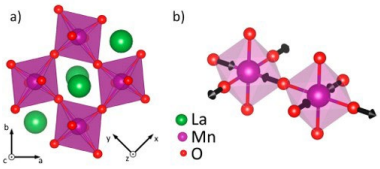
The **TACO Colloquium** talks in the winter term 2026/27 will take place at the University of Vienna. We still need to reserve a room in Kolingasse. Nevertheless, we have already invited the following speakers (talks start at 5 pm):

Date	**Speaker**	**Title**
Oct. 5	Philipp Rahe (University of Osnabrück)	*tbd*
Nov. 16	Bjarne Kreitz (Georgia Institute of Technology)	*tbd*
Dec. 21	Giovanni Di Liberto (Uni Milano Bicocca)	*tbd*
Jan. 25	Ying Jiang (University of Beijing)	*tbd*

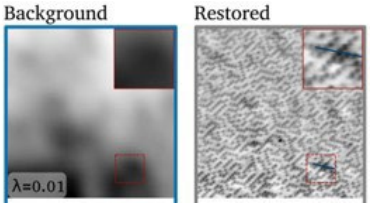
Thanks to everyone for their efforts to invite high-profile speakers!

3. TACO Papers

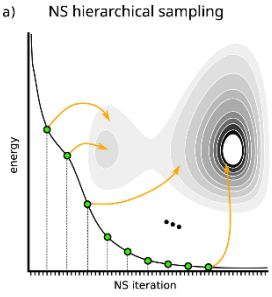
On the occasion of his 60th birthday, a Festschrift to honour Christoph Dellago appeared in *The Journal of Chemical Physics*. Christoph is one of the leading figures in the fields of statistical mechanics and molecular simulations, which he has shaped with lasting contributions. Accordingly, the Festschrift is titled "*Exploring Paths and Barriers in Statistical Mechanics*". Congratulations to Christoph on this rare event!



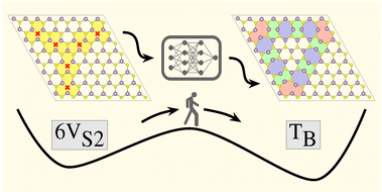
The best way to sample Christoph's path is by contributing to his Festschrift. This is what Cesare Franchini, together with three of his students, did with their paper "*Machine learning the order–disorder Jahn–Teller transition in $LaMnO_3$*". They investigated the Jahn-Teller structural phase transition in $LaMnO_3$ at $T_{JT} \simeq 750$ K using molecular dynamics simulations based on machine-learning force fields trained on *ab initio* data. Their results reproduce the experimental temperature dependence of both structural and phonon properties and highlight the presence of anharmonic effects at finite temperature.



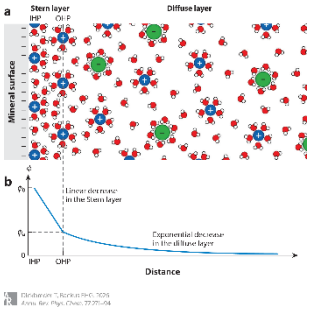
Marco Corrias, a former PhD student of Cesare Franchini in P07, is the first author of a joint TACO paper convening no less than three subprojects. In "*Total Variation-Based Image Decomposition and Denoising for Microscopy Images*", the authors from subprojects P07, P02, and P10 demonstrate a workflow to efficiently denoise microscopy images. The article appeared in the journal *Microscopy and Microanalysis*.



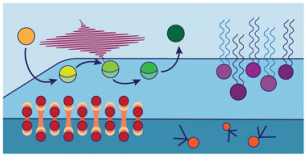
Newly graduated Nico Unglert successfully published in the journal *npj Computational Materials* in the *Nature* family. He published the article "*Active learning potentials for first-principles phase diagrams using replica-exchange nested sampling*" together with Michael Ketter and his PhD supervisor Georg Madsen. They present a fully automated active-learning strategy based on replica-exchange nested sampling for the generation of training data and the computation of complete pressure-temperature phase diagrams. The approach successfully reproduces known phase transitions of silicon, germanium, and titanium.



A second paper reported from subproject P09 is the article "*Completing the hierarchy of rotational defects in monolayer MoS2 through symmetry-aware evolutionary search*" by Alexander Adel, Ralf Wanzenböck, and Georg Madsen, published in *Physical Chemistry Chemical Physics*. The authors explore the three-fold rotational defect potential energy surface in the 2D material MoS_2 by combining an evolutionary algorithm with a machine-learning force field and report the discovery of several novel structures with reasonable computational effort.



The subproject P11 has also published two papers. The first one is a review about "*Interactions at Aqueous Mineral Interfaces: Insights from Nonlinear Optical Spectroscopy and Atomic Force Microscopy*" by Tobias Dickbreder and Ellen Backus. The comprehensive work appeared in the *Annual Reviews of Physical Chemistry*.



The second P11 paper is the introductory chapter to the *Faraday Discussion* "*Vibrations at Interfaces*". Ellen Backus and her team of authors discuss selected examples to highlight how the challenges that vibrational spectroscopy faces can be overcome to study interfaces and which research questions can be answered.

Congratulations to all authors! Please report any new publications to the science manager to keep the TACO publication list up to date.

4. New Projects and Grants

Florian Kraushofer, Co-PI with Gareth Parkinson in P04, received a principal-investigator grant worth 452 k€ for "*Modelling Single Atom Catalysts in Realistic Conditions*" from the Austrian Science Fund FWF. Georg Madsen will be a national cooperation partner, and Barbara Lechner from TU Munich an international cooperation partner. Congratulations!

5. Awards and Achievements

No new awards or achievements were reported in the past period. Surely, your next award is only around the corner!

6. Miscellaneous

The video of the TACO Colloquium talk by Taro Hitosugi (University of Tokyo) about "*Autonomous Experiments for Solid Materials: From Thin Films to Bulk Synthesis*" is newly available on our YouTube channel. Enjoy!

Videos of other colloquia talks are still in the making. Stay tuned, and subscribe to the channel!

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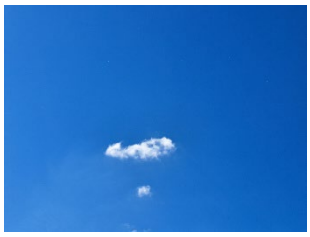

Bluesky:

https://bsky.app/profile/taco-oxides.bsky.social

YouTube:

https://www.youtube.com/@TACO_Oxides

7. Research fish reporting

To ease the collection of information for the annual and final status reports in Research fish required by our funding agency, the FWF, you are encouraged to report the following items to this new section of the TACO Newsletter:

- Collaborations & Partnerships
- Next Destination (i.e., career development of former TACO members)
- Research Tools & Methods
- Research Datasets, Databases & Models
- Intellectual Property & Licensing
- Software & Technical Products
- Use of Facilities & Resources

Please contact the Science Manager, Stefan Uttenthaler, to report items or if you have questions about what to report.