Christoph Dellago giving his family lecture in physics at the Long Night of Research on April 24.

TACO Newsletter

No. 04, August 2026

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Reporting period: June – July 2026

1. Personnel Developments

We welcome several new people to TACO.

Wenshan Chen is a new associated postdoc in Ulrike Diebold's subproject P02. In collaboration with an industrial partner, Wenshan optimises thin-film growth using pulsed laser deposition and surface-science techniques.

Similarly, Michael Sahre is an associated postdoc in Georg Kresse's subproject P03. Michael also participated in the TACO PhD Meeting in April. He will soon become a regular TACO member by moving to the TACO payroll.

Also, Michael Sachs is a new associated postdoc in Ellen Backus' subproject P11. Michael moved from Stanford University to Vienna, and you might have met him at the TACO PhD Meeting in April, where he spontaneously chaired a session.

Two new people joined Christoph Dellago's subproject P12. One of them is Marco Janach, who is a new PhD student and whom you might have met at the TACO PhD Meeting in April.

Finally, Maximilian Negledy is a PhD student newly associated with P12. You might have met him at the TACO PhD Meeting, where he gave a talk about "*Correlation-Free and Parallelizable Transition Path Sampling through Generative Committor Learning*".

While some people are joining, others are leaving – but not without celebrating academic successes! On June 3, Parinya "Lewis" Tangpakonsab successfully defended his thesis "*First-Principles Modeling of Oxide and Metal–Oxide Catalysts: Rationalizing Experimental Observations of CO, H_2, and CH_4 Oxidation*". His supervisors were Günther Rupprechter and Alexander Genest, both from subproject P08. Lewis continues to work as a postdoc in Günther's group while applying for postdoc positions. Congratulations, Dr Lewis!

On June 11, Alexandra Imre successfully defended her thesis "*Computational Methods for Surface Structure Optimization in LEED I (V)*". The picture features Alex with the examiners Georg Held and Florian Libisch, together with Alex' supervisor Ulrike Diebold. Congratulations, Dr Alex!

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

2. Upcoming Events

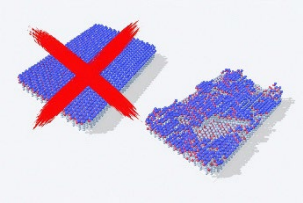
The **TACO Retreat** will take place at the Steinschalerhof in Rabenstein an der Pielach from **September 28 to 30, 2026**. The invited keynote speakers will be: **Gustav Bihlmayer**, **Stefan Blügel** (both Forschungszentrum Jülich), **Claudia Draxl** (HU Berlin), **David Duncan** (University of Nottingham), **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 Kolingasse 14-16, University of Vienna. The first talk will take place in room PC3; the remaining talks will take place in SR18. All talks start at 5 pm. Note that the colloquium by Bjarne Kreitz was shifted by one week compared to the previous announcement.

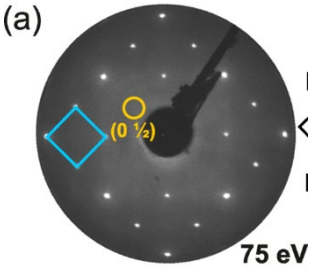
Date	Speaker	Title
Oct. 5	Philipp Rahe (University of Osnabrück)	*tbd*
Nov. 23	Bjarne Kreitz (Georgia Institute of Technology)	*tbd*
Dec. 21	Giovanni Di Liberto (Uni Milano Bicocca)	*tbd*
Jan. 25	Ying Jiang (University of Beijing)	*tbd*

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

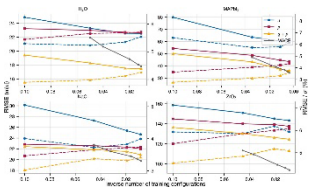
3. TACO Papers



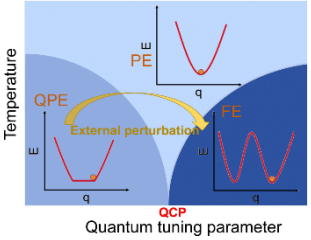
Many new TACO papers have been published in the reporting period. Two of them come from Ulrike Diebold's P02. The first one by Johanna Hütner-Reisch et al. directly reports its results in its title "*AFM imaging reveals the unreconstructed α-Al_2O_3(0001) surface to be inhomogeneous and rough*". The work appeared in the high-profile journal *Nature Communications* and was also featured in a TU Wien press release.



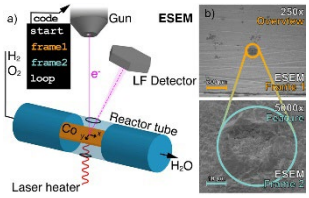
"*When surface dynamics fakes symmetry: Oxygen on Rh(100) revisited*" is the title of the second P02 paper, led by first-author Lutz Hammer. P02 PI Ulrike Diebold and Co-PI Michael Schmid are co-authors. In their article published in *Physical Review Research*, they show that heating a long-range ordered adsorbate phase beyond its stability temperature does not necessarily result in a disordered phase. Instead, it can break up into highly fluctuating ordered domains, which may give the impression of both an incorrect periodicity and false symmetry elements when averaging over larger areas or long time scales.



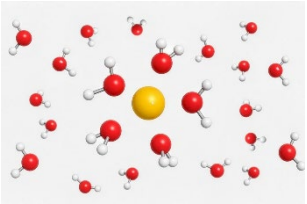
Bernhard Schmiedmayer from P03 introduced an alternative strategy for machine-learning tensorial quantities based on scalar descriptors to replace tensorial descriptors. He published his results together with Georg Kresse and others in the article "*Scalar machine learning of tensorial quantities—Born effective charges from monopole models*", which appeared in *The Journal of Chemical Physics*.



P07 PI Cesare Franchini, together with co-authors from the University of Vienna, Shanghai University, and the University of Bologna, once more targeted the favourite TACO material $KTaO_3$. They investigated the "*Emergent ferroelectric order in strained $KTaO_3$ by anharmonic and machine learned force fields methods*". The authors published their results in the journal *Physical Review Materials*.



Johannes Zeininger and Günther Rupprechter, both from P08, contributed to the article "*Multiscale Microscopy via Automation: Dual Magnification Environmental Scanning Electron Microscopy Imaging by Frame Alternation*", which appeared in the journal *Advanced Materials Technologies*. The work introduces an automation interface to minimise human intervention in environmental scanning electron microscopy experiments to maintain the image quality. The more advanced acquisition programs allow dual-magnification imaging to bridge length scales and capture the same process at the same location at different magnifications.



Finally, a paper emerged from a collaboration between subproject P11 (Ellen Backus and Moritz Zelenka) and the Valtiner group at the Institute of Applied Physics at TU Wien that was published in *Science Advances*. In their article "*Entropic-dielectric interplay governs ion adsorption in inner electric double layers*", the authors investigated how easily charged particles can be held at a surface. Water forms structures on nanosecond timescales that are statistical in nature. Some ions, such as lithium and calcium, more strongly influence the order of the surrounding water molecules. Thus, not only must electric charges be taken into account to understand the behaviour of the ions, but also the statistical order, the entropy, of water. The authors also presented a quantitative thermodynamic model to describe the interaction of ions in water with a charged surface. Also, this article was featured in a TU Wien press release.

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

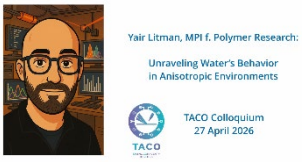
No new projects or grants were approved in the reporting period – at least none that we already may announce! ;-)

5. Awards and Achievements

Johanna Carbone, Co-PI of subproject P07, has been nominated as a member of the Psi-K working group D, “Wider Engagement”, Section 2, “Early career researchers” (including networking and mentoring). Congratulations, Johanna!

6. Miscellaneous

The last TACO Newsletter edition failed to report that many TACO people actively engaged in the Long Night of Research on April 24 to communicate their science to the public. A large group of people was active at TU Wien at Getreidemarkt. The picture features Ralf Wanzenböck, who showcased to a young audience the wonders liquid nitrogen can do. At the University of Vienna, Tobias Dickbreder and Ellen Backus demonstrated light and spectroscopy at the Faculty of Chemistry, while Moritz Zelenka and Sophie Zeilinger presented at the science market at the main building of the University. Finally, Christoph Dellago once more delivered his engaging family lecture at the Faculty of Physics of the University of Vienna; see the picture on the front page!



We have three new videos on our TACO YouTube channel! The first one is the colloquium talk by Yair Litman (Max Planck Institute for Polymer Research) about "*Unraveling Water's Behavior in Anisotropic Environments*".

Also, the video of the talk by Paul Erhart (Chalmers University of Technology) about "*The Interplay of Dynamics and Order in Mixed Perovskites*" went live.

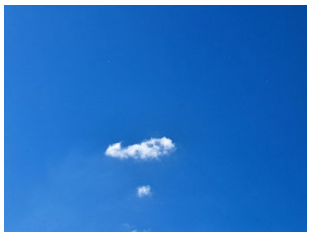
Finally, the latest addition to the TACO YouTube channel is the colloquium talk by Reinhard Maurer (University of Vienna) about "*Ultrafast Dynamics at Surfaces with Machine Learning Surrogates*".

Enjoy all of them!

Please follow our social media accounts and like & share content:

LinkedIn:

https://www.linkedin.com/company/taco-taming-complexity-in-materials-modeling/?viewAsMember=true



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.