

TACO Newsletter

No. 02, April 2026



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Reporting period: February – March 2026

1. Personnel Developments



No personnel developments were reported in February and March. Please inform the TACO science manager, [Stefan Uttenthaler](#), about personnel developments in your subproject.

2. Upcoming Events



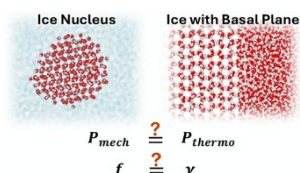
The **TACO PhD Meeting 2026** will take place at the [Seminar and Resort Hotel Flackl](#) in Reichenau an der Rax. The meeting is scheduled from **April 8 to 10, 2026**. The Scientific Organising Committee, comprising [Faith Lewis](#) (P04), [Susanne Gross](#) (P08), and [Tobias Dickbreder](#) (P11), has successfully attracted a suite of excellent external speakers. These will be (in alphabetical order): **Andrea Auer** (University of Innsbruck), **Sara Blomberg** (Lund University), **Rachael Farber** (University of Kansas), **Erin Iski** (University of Tulsa), **Bernhard R. Reischl** (University of Helsinki), and **Zbigniew Sojka** (Jagiellonian University, Krakow).

The **TACO Colloquium** talks in the summer term 2026 will take place again at TU Wien, in [Hörsaal 4](#) of the TU Freihaus (please follow the link to the location and directions to the lecture hall in the Freihaus). The talks start at 5 pm. The current schedule is as follows:

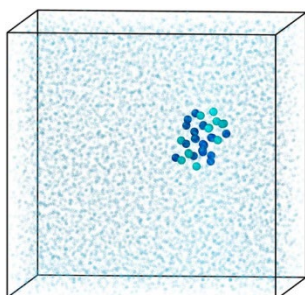
| Date | Speaker | Title |
|----------|---|---|
| April 27 | Yair Litman (MPI for Polymer Research) | Unraveling Water's Behavior in Anisotropic Environments |
| May 4 | Paul Erhart (Chalmers University of Technology) | <i>tbd</i> |
| June 1 | Reinhard Maurer (University of Vienna) | <i>tbd</i> |

The TACO science manager gladly accepts speaker suggestions for the winter term 2026/27!

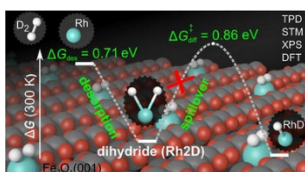
3. TACO Papers



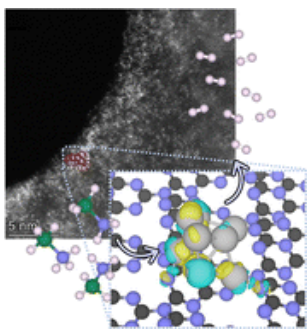
[Pablo Montero de Hijes](#), a postdoc with [Christoph Dellago](#) in P12, has already published two papers in 2026, both of them on the nucleation of ice. The first one, published in *The Journal of Physical Chemistry Letters*, is “[Comparing the Mechanical and Thermodynamic Definitions of Pressure in Ice Nucleation](#)”. Pablo and his co-authors find that, unlike in hard-sphere and Lennard-Jones systems, mechanical and thermodynamic pressures agree for the nucleus, and the interfacial stress and free energy are comparable. However, the basal interface displays an interfacial stress nearly twice its interfacial free energy, suggesting that this agreement may depend on the system, underscoring the limitations of mechanical routes to solid–liquid interfacial free energies.



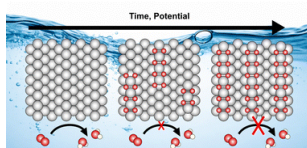
In the second paper, published in *The Journal of Chemical Physics*, [Pablo](#) and his co-authors [Sebastian Falkner](#) and [Christoph Dellago](#) investigated “[Non-Markovian dynamics in ice nucleation](#)”. In other words, they investigated, for the case of homogeneous ice nucleation, whether the nucleus size exhibits Markovian dynamics, as assumed in classical nucleation theory. With their work, they establish an improved reaction coordinate compared to the size of the largest crystalline nucleus, and they test it for Markovian dynamics.



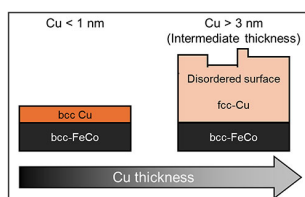
The article “[Hydrogen Activation via Dihydride Formation on a Rh₁/Fe₃O₄\(001\) Single-Atom Catalyst](#)” by [Chunlei Wang](#) and Panukorn Sombut et al. is a joint paper with contributions from three TACO subprojects, namely P02 ([Ulrike Diebold](#)), P04 ([Gareth Parkinson](#)), and P07 ([Cesare Franchini](#)). Using an armada of experimental techniques, the authors show that isolated Rh adatoms supported on Fe₃O₄(001) activate hydrogen by forming a stable dihydride species without atomic H spillover. DFT-based and random-phase-approximation calculations provide further insight into the process. The article was published in *Angewandte Chemie International Edition*.



A paper coming out from [Karin Föttinger](#)'s subproject P10 investigates the "[Influence of nitrogen functional groups in carbon-based supports anchoring Pt nanoclusters and single atoms for efficient ammonia borane hydrolysis](#)". Ilaria Barlocco and collaborators published their work in the journal *Chemical Communications*. Well done!



Two more papers come out of [Ulrike Diebold](#)'s subproject P02. The first one, published by Larsson et al. in the journal *EES Catalysis*, investigates how "[Platinum surface oxides govern the cathodic overpotential of the oxygen reduction reaction](#)". It illustrates how oxides inhibit the oxygen reduction reaction during fuel cell start-up. Crucially, the authors demonstrate that the ORR onset is delayed until these oxides are reduced.



Finally, Takezawa et al., with contributions from [Michele Riva](#), [Florian Dörr](#), and [Michael Schmid](#) (all from P02), inspected the "[Initial Growth Process of Cu Thin Films on bcc-FeCo/MgO\(100\) via Molecular Beam Epitaxy](#)". For very thin films (<1 nm), Cu adopted a body-centred cubic structure templated by the underlying FeCo substrate. Once the Cu thickness exceeded approximately 3 nm, a structural transformation into the face-centred cubic phase was observed. In this thickness range, the MBE-grown films exhibited interfacial dislocations and developed a disordered surface. The article was published in the *e-Journal of Surface Science and Nanotechnology*.

Please report any new publications to the science manager to keep the [TACO publication list](#) up to date.

4. New Projects and Grants



dataTUdiscovery

The fuTUre fit project [dataTUdiscovery](#), led by P09 Co-PI [Esther Heid](#), has commenced. It is among the eleven funded large fuTUre fit projects and will bring AI/ML support to all research groups at TU Wien. You are welcome to apply for project positions!

5. Awards and Achievements



TACO Co-PI [Esther Heid](#) (P09) was elected a member of the [Young Academy](#) of the Austrian Academy of Sciences (ÖAW). Together with 45 additional newly elected members, she will strengthen the ÖAW in the future. Congratulations, Esther!



[Georg Madsen](#)'s subproject P09 has one more success story to offer: PhD student [Eva Doloszeski](#) received a [Marietta Blau Grant](#) from Austria's Agency for Education and Internationalisation (OeAD). She will use the grant for a seven-month research stay at Aarhus University in the group of [Bjørk Hammer](#), a member of the TACO Scientific Advisory Board. Starting from April, Eva will research the uncertainty quantification in atomistic foundation models. Congratulations, Eva!

6. Miscellaneous



Hans-Peter Steinrück,
FAU Nürnberg:
Ionic Liquid Interfaces



TACO Colloquium
26 January 2026

We have one new video of a colloquium talk on our YouTube channel: Hans-Peter Steinrück (FAU Erlangen-Nürnberg) presented “[Ionic Liquid Interfaces](#)” in January. You can now re-watch the talk on YouTube!

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



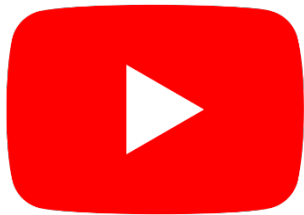
LinkedIn:

<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.