

**TACO Newsletter**  
**No. 06, December 2025**



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Reporting period: October – November 2025

## 1. Personnel Developments



[Michael Pittenauer](#), TACO PhD student in subproject P10 with [Karin Föttinger](#), successfully defended his thesis titled „Selective oxidation of 2-propanol on cobalt and nickel ferrite nanoparticles” on October 16. He has been working at the company KremsChem since the beginning of March 2025. Congratulations, Dr Michael!



On November 20, TACO PhD student [Marco Corrias](#) successfully defended his PhD thesis titled “Computer Vision and Machine Learning Analysis of Atomic-Scale Microscopy Images”. Pictured here, Marco (centre) can be seen with (from left to right) his PhD supervisor [Cesare Franchini](#), Stefan Förster (external examiner and invited speaker at the first TACO PhD Meeting 2022), Thomas Pichler (committee head, University of Vienna), and Luca Ghiringhelli (external examiner). Congratulations, Dr Marco!

Please inform the TACO science manager, [Stefan Uttenthaler](#), about personnel developments in your subproject.

## 2. Upcoming Events



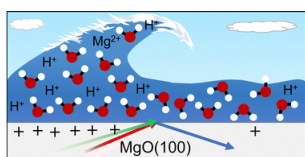
The **TACO PhD Meeting 2026** will take place at the [Seminar and Resort Hotel Flackl](#) in Reichenau an der Rax. The meeting is scheduled from **April 8 to 10, 2026**. The Scientific Organising Committee, comprising [Faith Lewis](#) (P04), [Susanne Gross](#) (P08), and [Tobias Dickbreder](#) (P11), has already 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), **Marie-Pierre Gaigeot** (Université d'Evry Val d'Essonne, Paris), **Erin Iski** (University of Tulsa), and **Zbigniew Sojka** (Jagiellonian University, Krakow). The PIs and Co-PIs have already been asked to name participants from their groups.

Two more **TACO Colloquia** are scheduled for the winter term 2025/26, which will take place in Lecture Room 2 of the Chemistry Department at the University of Vienna, located at Währingerstraße 42.

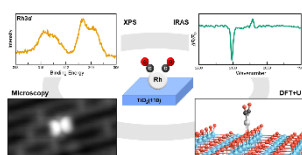
The colloquium talks in the summer term will take place again at TU Wien; the room still needs to be booked. The dates of two speakers have already been fixed, and two more appointments are planned.

Date	Speaker	Title
<b>Winter term</b>		
Dec. 15	<a href="#">Albert Bartok-Partay</a> (University of Warwick)	<i>Materials Modelling Across the Scales</i>
Jan. 26	<a href="#">Hans-Peter Steinrück</a> (FAU Erlangen-Nürnberg)	<i>Ionic Liquid Interfaces</i>
<b>Summer term</b>		
Mar. 23	<a href="#">Taro Hitosugi</a> (University of Tokyo)	<i>Autonomous Experiments Driven by Machine Learning and Robots</i>
Apr. 27	<a href="#">Yair Litman</a> (MPI for Polymer Research)	<i>tbd</i>

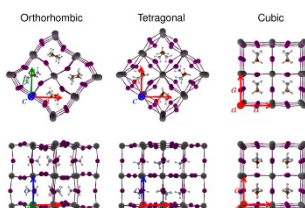
### 3. TACO Papers



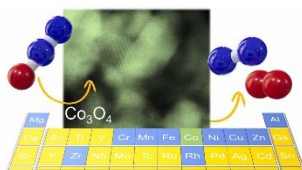
In a paper published by [Moritz Zelenka](#) and [Ellen Backus](#) (both P11) in the journal *Physical Chemistry Chemical Physics* in October, they report that at the “[MgO–water interface, structure and surface dissolution depend on flow and pH](#)”. Moritz and Ellen explain this surprising observation with the dissolution of MgO in aqueous solutions, which effectively removes charge from the interfacial region. Other solid–liquid interfaces with similar or higher solubility might exhibit similar properties.



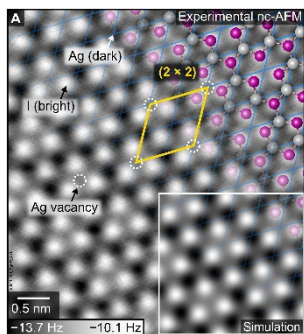
A team of authors from as many as three TACO subprojects, namely P04, P02, and P07, published the article “[Multi-technique characterization of rhodium gem-dicarbonyls on TiO<sub>2</sub>\(110\)](#)” in the journal *Chemical Science* in October. [Moritz Eder](#) et al. combined spectroscopy, scanning probe microscopy, and DFT calculations to determine the location and coordination of the rhodium gem-dicarbonyls on a single-crystalline rutile TiO<sub>2</sub>(110) on the surface. The results highlight the complex behaviour of carbonyls on metal oxide surfaces, and demonstrate the necessity of multi-technique approaches for the adequate characterisation of single-atom catalysts.



[Bernhard Schmiedmayer](#), PhD student in [Georg Kresse](#)'s subproject P03, is the first author of the article “[Equivariant machine learning of electric field gradients—Predicting the quadrupolar coupling constant in the MAPbI<sub>3</sub> phase transition](#)”, which was published in *The Journal of Chemical Physics*. The authors present a new strategy that combines machine learning and first-principles calculations to achieve highly accurate predictions of nuclear quadrupolar coupling constants.



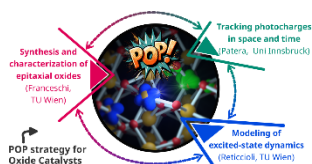
A team of authors, including [Silvio Bellomi](#) and [Karin Föttinger](#) from subproject P10, presented a “[Comparative study of multi-element modification and rhodium promotion of Co<sub>3</sub>O<sub>4</sub>-based spinel catalysts for N<sub>2</sub>O decomposition](#)” in the journal *Applied Catalysis A: General*. Catalysts obtained from Co<sub>3</sub>O<sub>4</sub> by the addition of Al or Rh emerged as the most active catalyst for the conversion of the environmentally problematic N<sub>2</sub>O.



The article “[Surface reconstructions govern ice nucleation on silver iodide](#)”, with participation of [Ulrike Diebold](#) and [Michael Schmid](#) from subproject P02, and [David Kugler](#) from P04, appeared in *Science Advances*. The work revealed the microscopic details of ice crystal formation on the surface of silver iodide, which is often used in cloud seeding processes. These details had remained unclear for a long time. The authors report that silver iodide exposes two fundamentally different surfaces, but only one of them promotes ice nucleation. TU Wien issued a [press release](#) about the new work on its website.

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

## 4. New Projects and Grants



The proposal for the Research Group [“Pushing Oxide Catalysis: Atomic-Scale View at Photocharges \(POP\)”](#) by the former TACO Co-PI [Michele Reticcioli](#), Laerte Patera, TACO Colloquium speaker of December 2023, and Giada Franceschi, Elise-Richter fellow in the Surface Physics Group at TU Wien, has been approved by the FWF Scientific Board. [Carla Verdi](#), former P03 Co-PI and now a fellow at the Faculty of Science, University of Sydney, Australia, serves as one of the international cooperation partners. The total funding sum is 1.5 M€. Michele will move to TU Wien as the project PI. Congratulations to all successful PIs, and welcome back to Vienna, Michele!



P10 PI [Karin Föttinger](#) was highly successful in applying for funding: The Austrian Research Promotion Agency FFG approved the project proposals "Green Synergy" and "EASYHac – Electrochemical Acetic acid from Syngas and Hydrogen as co-product", the second of which is coordinated by the COMET competence centre [K1Met](#). The FWF, on the other hand, approved the project proposal [“TRANSFORM”](#) of PI Thomas Konegger, in which Karin is a cooperation partner. It is an international research project in cooperation with scientists in France, aimed at the *in situ* design of transition metal nanoparticles in micro- or mesoporous additively manufactured Polymer-Derived Ceramic parts for the production of value-added chemicals. Congratulations, Karin!

## 5. Awards and Achievements



No new awards or achievements were reported in the reporting period.

## 6. Miscellaneous



The TACO PhD dinner took place on November 26. The dinner was organised by the student representatives [Faith Lewis](#) and [Eva Doloszeski](#), and it was very popular: 18 young TACO scientists met at restaurant OTTO YAMI and discussed recent progress and new joint research projects! ;-)



The TACO women's lunch took place on December 1: The interaction between TACO PIs and junior researchers was very fruitful, and several new initiatives have been hatched – stay posted about the implementation! Our TACO women were too involved in discussions to take a photo. No problem nowadays, our Science Manager created a picture with AI (Adobe Firefly Image 5). The food came out nicer, the people perhaps not so much.

Several new talk videos went online on the TACO YouTube channel. These include all six invited keynote talks at the TACO Retreat, as well as the colloquium talk by Alec Wodtke. Follow the links to watch the talk videos.



Hannes Jónsson, University of Iceland: "[Towards Improved Methodology for Photocatalysis Simulations](#)";



Greg Kimmel, PNNL:  
The structure and reactivity  
of water and carboxylic acids  
on model TiO<sub>2</sub> catalysts  
TACO Retreat  
22 September 2025

Greg Kimmel, Pacific Northwest National Laboratory: [“The Structure and Reactivity of Water and Carboxylic Acids on Model TiO<sub>2</sub> Catalysts”](#);



Lorenzo Monacelli,  
University La Sapienza:  
Quantum Simulations of Ions  
TACO Retreat  
23 September 2025

Lorenzo Monacelli, University La Sapienza: [„A Unified Quantum Framework for Electrons and Ions: The Self-Consistent Harmonic Approximation on a Neural Network Curved Manifold”](#);



Benjamin Rotenberg,  
Sorbonne University:  
Making Sense of Electrical Noise  
by Simulating Electrolyte Solutions  
TACO Retreat  
23 September 2025

Benjamin Rotenberg, Sorbonne University: [„Making Sense of Electrical Noise by Simulating Electrolyte Solutions”](#);



Alexander Ganose,  
Imperial College London:  
Electron and Thermal Transport  
at Database Scale  
TACO Retreat  
24 September 2025

Alexander Ganose, Imperial College London: [“Electron and Thermal Transport at Database Scale”](#);



Johannes Margraf,  
University of Bayreuth:  
How Foundation Models  
for Atomistic Modelling  
are Changing Materials Discovery  
TACO Retreat  
24 September 2025

Johannes Margraf, University of Bayreuth: [“How Foundation Models for Atomistic Modelling are Changing Materials Discovery”](#);



Alec Wodtke,  
MPI for Multidisciplinary Sciences:  
Bridging the Pressure Gap  
in Heterogeneous Catalysis  
TACO Colloquium  
06 October 2025

Alec Wodtke, Max Planck Institute for Multidisciplinary Sciences: [“Bridging the Pressure Gap in Heterogeneous Catalysis”](#);

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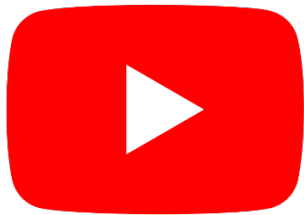
LinkedIn:

<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](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.