Group picture of the TACO Retreat 2025 in Steinschaler Dörfl, Frankenfels.

TACO Newsletter

No. 05, October 2025

Content

Reporting period: August – September 2025

1. Personnel Developments

Moritz Zelenka from Ellen Backus' subproject P11 successfully defended his PhD thesis on September 29. The thesis title is "*The Molecular Structure at Solid-Liquid Interfaces: From Surface Dissolution to Heterogeneous Catalysis*". He will stay in Ellen's group as a PostDoc and continue to work on TACO topics, funded by the University of Vienna. Congratulations, Dr. Zelenka!

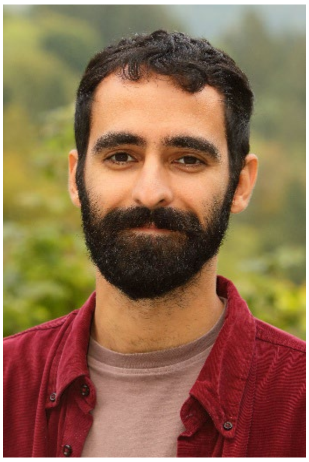
Christian Schäfer is a new tenure-track Assistant Professor in the surface science group at TU Wien and is associated with Gareth Parkinson's subproject P04. Christian gave a talk at the TACO Retreat 2025 about "Taming Polaritonics". Welcome to TACO, Christian!

Daniela Mangano is a new PhD Student in Cesare Franchini’s subproject P07. You might have made her acquaintance at the TACO Retreat 2025. Welcome to TACO, Daniela!

Also, Luca Leoni is a new PhD Student associated with Cesare Franchini’s subproject P07. You might have met Luca at the TACO Retreat 2025, where he presented a poster with the title “*Machine Learning Potentials for Localized Charge Dynamics in Materials*”. Welcome to TACO, Luca!

Darin Joseph is the third new PhD Student associated with Cesare Franchini’s subproject P07. You might have met him at the TACO Retreat 2025. Welcome to TACO, Darin!

Jakub Szmitek is a new PhD Student in Georg Madsen's subproject P09 who also attended the TACO Retreat. Welcome to TACO, Jakub!



Gustavo Andrade Silva Alves is a new PhD Student in Karin Föttinger's subproject P10. Gustavo attended the TACO Retreat 2025, where he presented a poster with the title "*MoS_2 Catalysts for CO_2 Hydrogenation to Methanol: Investigating the Interplay between Oxides and Sulfides via In-situ X-Ray Absorption Spectroscopy*". Welcome to TACO, Gustavo!

Sophie Zeilinger is a new student in Ellen Backus' subproject P11. She is currently preparing to finish her master's thesis and will then join TACO as a PhD Student. Sophie already attended the TACO Retreat 2025, where she presented a poster with the title "*SAXS Analysis of Fluorinated Acid-Induced Microheterogeneties in HFIP Water Binary Mixtures*". Welcome to TACO, Sophie!

Finally, Justin Pils is a new student in Christoph Dellago's subproject P12. Justin also attended the recent TACO Retreat and will become a PhD Student soon. Welcome to TACO, Justin!

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 **TACO Colloquium** schedule for the winter term 2025/26 has been established. Alec Wodtke (MPI for Multidisciplinary Sciences) already presented *"Bridging the Pressure Gap in Heterogeneous Catalysis"* on October 6. The following three additional talks will take place in lecture room 2 in the Chemistry Department of the University of Vienna in Währingerstraße 42.

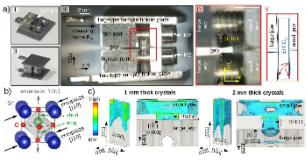
Date	Speaker	Title
Nov. 24	Marc Koper (Leiden University)	*Electric Double Layer of Platinum Electrodes*
Dec. 15	Albert Bartok-Partay (University of Warwick)	*tbd*
Jan. 26	Hans-Peter Steinrück (FAU Erlangen-Nürnberg)	*Ionic Liquid Interfaces*

3. TACO Papers

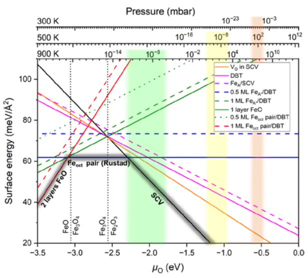
Please be reminded that the FWF requires us to put the following text in our open-access TACO publications:

"This research was funded in whole or in part by the Austrian Science Fund (FWF) [10.55776/F8100](10.55776/F8100). For open access purposes, the author has applied a CC BY public copyright license to any author accepted manuscript version arising from this submission."

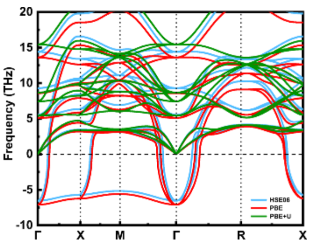
You may choose to delete "in whole" or "in part", depending on what is the actual case. You do not need to be creative beyond this!



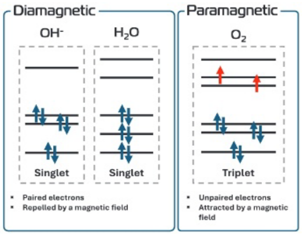
Earlier this year, Igor Sokolović, Michael Schmid, Ulrike Diebold (subproject P02), and their collaborator Martin Setvín demonstrated a new method of "*How to cleave cubic perovskite oxides*". They discuss a method for strain-assisted cleaving of perovskite single crystals on the model cubic perovskite oxide $SrTiO_3$(001) and show that it also works on $KTaO_3$(001) and $BaTiO_3$(001). This approach opens up a pathway for obtaining high-quality surfaces of this promising class of materials.



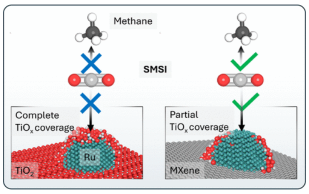
A team behind first author Panukorn Sombut, including Michael Schmid and Ulrike Diebold from P02, Moritz Eder and Gareth Parkinson from P04, and Matthias Meier and Cesare Franchini from P07, revisited "*The surface phase diagram of Fe_3O_4(001)*". The authors computed the surface phase diagram of the Magnetite (001) facet using DFT-based calculations, with an emphasis on understanding the terminations observed in surface science experiments. Their results reveal two stable terminations.



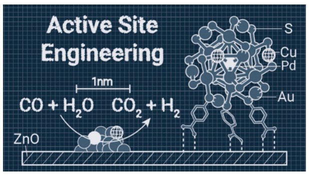
Darin Joseph and Cesare Franchini from subproject P07 investigated the formation of electron and hole small polarons in the prototypical ferroelectric material $BaTiO_3$. In their article titled "*Coupling between small polarons and ferroelectricity in $BaTiO_3$*", they employ the HSE06 hybrid density functional, which addresses the limitations of conventional DFT models. The authors uncover the trend in electron-polaron stability in the cubic, tetragonal, and rhombohedral structural phases of $BaTiO_3$. The paper was published in the journal *Physical Review Materials* on September 30. Congratulations, Darin and Cesare!



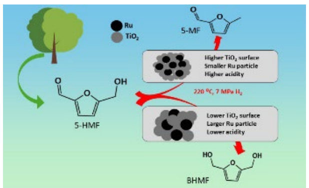
Cesare Franchini was also involved in writing of a review article on "*Spin Matters: A Multidisciplinary Roadmap to Understanding Spin Effects in Oxygen Evolution Reaction During Water Electrolysis*", which is relevant to TACO. The extensive article appeared in the journal *Advanced Energy Materials*. Well done, Cesare!



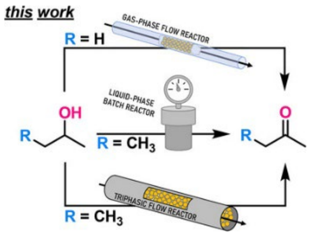
Thomas Wicht and Günther Rupprechter from P08, together with a few additional authors, presented their article "*Influence of MXene and TiO_2 on the Performance of Microalgae-Derived Ru-Based Catalysts for CO_2 Hydrogenation to Methane*" in the journal *ACS Catalysis*. This work addresses the challenge of controlling the selectivity of CO_2 hydrogenation to produce value-added fuels and chemicals by catalysis. Indeed, Ru/MXene exhibited superior catalytic activity after reductive pretreatment. Well done, Thomas and Günther!



Another piece of work that comes out of subproject P08 is the article "*Engineering Catalytic Efficiency by Thiolate-Protected Trimetallic (Cu, Pd, Au) Nanoclusters: Single-Atom Alloy Catalysts for Water–Gas Shift*". Here, Thomas Haunold and Günther Rupprechter are among the authors. The authors conclude that the thiolate-protected single-atom alloy nanoclusters may become industrially relevant when upscaled while still serving as a well-defined model system in catalysis. The article appeared in *ACS Catalysis* in August. Congratulations to Thomas and Günther!



Two papers also come out of Karin Föttinger's subproject P10. The first one investigated the "*Switchable Behavior of Ru–TiO_2 Catalysts in HMF Conversion*". The current P10 PhD student Gustavo Andrade Silva Alves and the former TACO postdoc Alberto Tampieri are also among the authors. This study revealed the switchable behavior of Ru/TiO_2 catalysts (anatase- and rutile-dominant) and exposed the critical role of TiO_2 structural and morphological features for reaction pathways in 5-Hydroxymethylfurfural valorization over Ru/TiO_2.



Finally, Alberto Tampieri et al., including PhD student Michael Pittenauer and Karin Föttinger, explored the "*Phase-Dependent Catalytic Oxidation of Secondary Alcohols Using Spinel Cobaltite Catalysts Under Liquid- and Gas-Phase Flow Conditions*". The "spongy" catalysts such as Co_3O_4, $MnCo_2O_4$, $NiCo_2O_4$, $ZnCo_2O_4$, and $CoFe_2O_4$ were synthesised by combustion, the process of which can be watched in a video with Alberto. Gas phase reactions unveiled the different behavior of the same catalysts in different environments, highlighting phase-specific effects such as the beneficial (liquid phase) versus inhibiting (gas phase) impact of Mn doping.

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

4. New Projects and Grants

No newly funded projects or grants were reported. Nevertheless, several ERC grants from our group have been submitted – let's keep our fingers crossed for the applicants!

5. Awards and Achievements

Susanne Gross from Günther Rupprechter’s subproject P08 received a Dieberger-Skalicky Stipend for PhD students in the academic year 2025/26. The 4,000 EUR stipend supports expenses related to research work, including scientific publications, material costs, laboratory equipment, research stays abroad, and conference participation. Congratulations, Susanne!

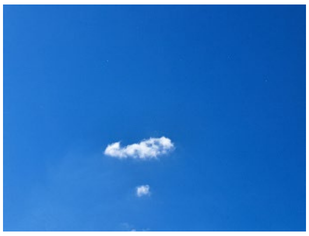
6. Miscellaneous

No new talk videos have been published on our TACO YouTube channel in the reporting period. However, the recordings of the invited talks at the TACO Retreat will be processed soon. Keep an eye on new videos that might appear on our channel soon!

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.