



The FWF Scientific Board approved our proposal for the second funding period!

TACO Newsletter

06/2024

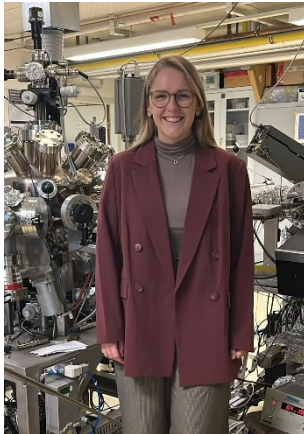


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Reporting period: October – November 2024

1. Personnel Developments



[Marie Kienzer](#) from Ulrike Diebold's subproject P02 recently finished her master's studies and graduated to "Diplom-Ingenieur". She is pictured here with the machine on which she did the experiments for her thesis. She will continue to work in TACO as a PhD student as of December 1. Congratulations, DI Marie!



[Ralf Wanzenböck](#) successfully defended his PhD thesis on October 30th. The former PhD student of subproject P09 is pictured here with one of his examiners and two supervisors. Ralf received a Senior Scientist position at TU Wien and now continues to work on TACO-related topics. Congratulations, Dr. Ralf!

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

2. Upcoming Events



The **TACO PhD Meeting 2025** will take place again in Schladming, but unlike in the last years, we will stay in **Sporthotel Royer** this time. We have reserved rooms for **February 2 to 5, 2025**. The SOC, composed of the junior TACO scientists [Bernhard Schmiedmayer](#), [Alessandro Coretti](#), and [Qaisar Magbool](#), is currently inviting speakers and preparing the program.



Mark your Calendar: The **TACO Retreat 2025** will take place again in **Steinschaler Dörfel** from **September 22 to 24, 2025**.

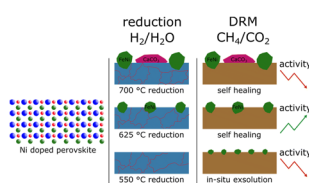
The **TA[CO]lloquium** schedule for fall and winter 2024/2025 is given below. The talks will take place again at the University of Vienna, Kolingasse 14-16 (in SR 9 and PC-SR 3, respectively).

Date	Speaker	Title
Nov 04	Xavier Gonze (UC Louvain, Belgium)	<i>Electron-Phonon Interaction: Band-Gap Renormalization, High-Throughput Analysis of Polaron Models, Contribution to Total Energy</i>
Dec 16	David Kubička (University of Chemistry and Technology Prague)	<i>The Peculiar Role of Supports in the Hydrogenation of Biomass-Derived Oxygenates</i>
Jan 13	Sereina Riniker (ETH Zurich, Switzerland)	<i>Learning Physical Interactions for Molecular Dynamics Simulations</i>
Jan 27	Karsten Reuter (Fritz Haber Institute, Germany)	<i>tbd</i>

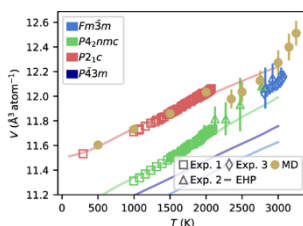
3. TACO Papers



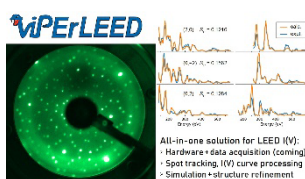
Below, a selection of recent TACO papers is reported.



[Florian Schrenk](#) et al. from Karin Föttinger's subproject P10 published a work on [“How reduction temperature influences the structure of perovskite-oxide catalysts during the dry reforming of methane”](#) in *RSC Sustainability*. It is part of the themed collection on CO₂ Conversion. Congratulations to the team!



A new paper came out from P09: [Georg Madsen](#) and [Jesús Carrete](#) published together with their PhD student and first author Sebastian Bichelmaier in the Journal *Physical Review B*. The article presents a [“Neural network enabled molecular dynamics study of HfO₂ phase transitions”](#). Well done!



The yearlong efforts by TACO scientists in P02 to make LEED a more user-friendly tool have finally reached a milestone. Two papers describing the ViPERLEED package have recently been accepted for publication in *Physical Review Research*. The first one by Florian Kraushofer et al. is on the [“Calculation of I\(V\) curves and structural optimization”](#), the second one by Michael Schmid deals with the [“Spot tracking, extraction and processing of I\(V\) curves”](#). The authors are currently working on the proofs, while the articles are already available on the arXiv. A text describing the works in some detail is in preparation for the TACO website.

The complete, up-to-date [TACO publication list](#) can be found on our website.

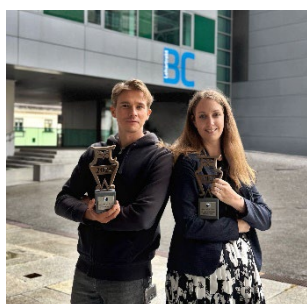
4. New Projects and Grants



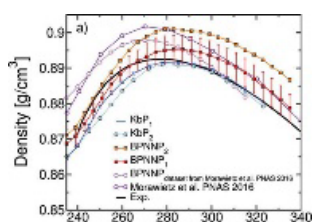
FWF Österreichischer
Wissenschaftsfonds

We can congratulate ourselves! Thanks to all your efforts and diligent work, the FWF's Scientific Board, in its meeting earlier this week, [approved our proposal](#) of four more years of human and artificial intelligence in TACO! The hearing on October 17 went smoothly and was successful. We expect to receive official confirmation letters and the extension contract before Christmas so that we can also extend employment contracts in due time.

5. Awards and Achievements



Congratulations once again to [Esther Heid](#)! She received [TU Wien's Best Teaching Award](#) in the category of Best Lecture together with Georg Ramer for their lecture "Programming for Chemists". She is pictured here with Alexey Cherevan, who won in the category of Best Teacher. Congrats!



The *Journal of Chemical Physics* article "[Comparing machine learning potentials for water: Kernel-based regression and Behler–Parrinello neural networks](#)" by [Pablo Montero de Hijes](#) and with co-authors [Christoph Dellago](#) (both P12), [Bernhard Schmiédmayer](#), and [Georg Kresse](#) (both P03) celebrates a nice success. The [extended press release](#) of this year's Nobel Prize in physics to John J. Hopfield and Geoffrey E. Hinton "for foundational discoveries and inventions that enable machine learning with artificial neural networks" cites the article for what studies are possible with these models. Let us celebrate this high recognition of their TACO work!

6. Miscellaneous



We have several new talk videos on our [TACO YouTube channel](#). You are invited to watch and learn from them.



Daniel Boese, Uni Graz:
Intermolecular Interactions:
Surfaces, Molecules,
and Molecular Crystals
TACO Colloquium
13 May 2024

Daniel Boese (TU Graz) gave a TA[CO]lloquium talk about “[Intermolecular Interactions: Surfaces, Molecules, and Molecular Crystals](#)” in May. The main findings presented therein have been published recently by Fishman et al. on the [arXiv](#).



Xavier Gonze, UC Louvain:
Electron-Phonon Interaction:
Band-Gap Renormalization,
High-Throughput Analysis
of Polaron Models,
Contribution to Total Energy
TACO Colloquium
04 November 2024

More recently, Xavier Gonze (UC Louvain) presented “[Electron-Phonon Interaction: Band-Gap Renormalization, High-Throughput Analysis of Polaron Models, Contribution to Total Energy](#)” at the TA[CO]lloquium.



Kieron Burke, UC Irvine:
Electronic Structure Calculations:
Past, Present, and Future
TACO Retreat
23 September 2024

Kieron Burke (UC Irvine) gave a keynote talk at the TACO Retreat about “[Electronic Structure Calculation: Past, Present, and Future](#)”.



Gregory Rohrer, Carnegie Mellon:
Modifying SrTiO₃ Surfaces
to Maximize
Photochemical Water Splitting
TACO Retreat
25 September 2024

Greg Rohrer (Carnegie Mellon University) also gave a keynote talk at the TACO Retreat. He presented “[Modifying SrTiO₃ Surfaces to Maximize Photochemical Water Splitting](#)”.

Enjoy the videos!