



# TACO Newsletter

## 03/2024



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Reporting period: April – May 2024

## 1. Personnel Developments



We welcome a couple of new outstanding people to TACO, some of which enter the project in preparation for the interim evaluation. Their profiles still have to be published on our website. Sorted by sub-project number, we welcome:



[Sylwia Gutowska](#) is the new Co-PI of Georg Kresse in sub-project P03 at the University of Vienna.



[Payal Wadhwa](#) has been a postdoc in P03 with Georg Kresse for a while already. Eventually, we can present her with a photo!



[Esther Heid](#) is the new Co-PI of Georg Madsen in sub-project P09 at TU Wien.



The fourth theoretician in the league is Alexander Gorfer, PhD student of Christoph Dellago in sub-project P12.

Welcome to TACO to all! We wish them much success with their research projects and studies!

Are there personnel developments in your TACO subproject? Tell the science manager, [Stefan Uttenthaler](#), about it!

## 2. Upcoming Events



In September, we will have another **TACO Retreat!** The dates are **September 23-25**, and we will be hosted again by Steinschaler Dörfel in Frankenfels, Lower Austria. We will have the following top-notch invited speakers: [Gregory S. Rohrer](#) (Carnegie Mellon University), [Alexandre Tkatchenko](#) (University of Luxemburg), [Marta Gibert](#) (TU Wien), [Paul A. Fenter](#) (Argonne National Laboratory), and [Kieron Burke](#) (UC Irvine). You can look forward to inspiring talks!

We will also use the retreat to prepare for the **FWF hearing** in the framework of the TACO interim evaluation. The hearing will take place on **Thursday, October 17**.

We are still in the making of the **TA[CO]lloquium** schedule for fall and winter 2024. The talks will take place again at the University of Vienna (room tbd). We have invited the following speakers and agreed dates with them:

<b>Date</b>	<b>Speaker</b>	<b>Title</b>
November 11	<a href="#">Xavier Gonze</a> (UC Louvain, Belgium)	<i>tbd</i>
January 27	<a href="#">Karsten Reuter</a> (Fritz Haber Institute, Germany)	<i>tbd</i>

We also fixed the date of the **TACO Ph.D. Meeting 2025**: It will be held from **February 2 to 5** (Sunday till Wednesday)! This time, we will stay in Sporthotel Royer, where we will only have single- and double-bed rooms.

### 3. TACO Papers



The following contains critical information regarding open-access fees for TACO publications.

At the end of last year, our funding agency FWF discontinued its Peer-Reviewed Publications program. The FWF replaced it with the Open-Access Block Grant, which the research institutions now administer. You can find details on the FWF website:

<https://www.fwf.ac.at/en/funding/portfolio/communication/open-access-block-grant>

As the FWF funds TACO, we are obliged to publish open access. The new Open-Access Block Grant has two crucial consequences for our publications:

1) We have to contact our universities for the payment of open-access fees. The contacts are [openaccess@univie.ac.at](mailto:openaccess@univie.ac.at) at the University of Vienna and [openaccess@tuwien.ac.at](mailto:openaccess@tuwien.ac.at) at TU Wien. It is recommended that you contact them early in the publication process, at the latest when you receive the invoice from the publisher. Never pay the invoice from a project or a private account! Refunds are not possible anymore!

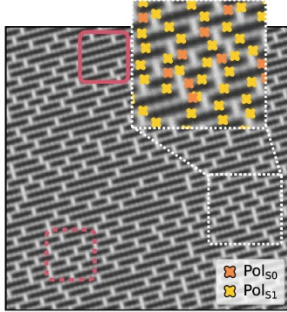
2) You must include the following text in all publications upon submission:

*“This research was funded in whole or in part by the Austrian Science Fund (FWF) 10.55776/F81. For open access purposes, the author has applied a CC BY public copyright license to any author accepted manuscript version arising from this submission.”*

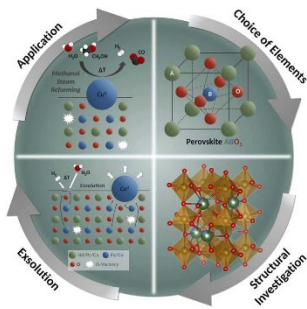
Here, 10.55776/F81 is the TACO grant DOI; see <https://www.fwf.ac.at/forschungsradar/10.55776/F81>. It is crucial to always apply a CC BY public copyright license to your publication to comply with the FWF open access policy. In the first sentence of the above text, you may choose the applicable option “in whole” or “in part”.

The deadline for the TACO interim proposal casts its shadows before and so there are many new TACO papers – too many to list them all here. The following is a (more or less random) selection of new papers the SFB manager was made aware of. The list is kept up to date on our [website](#).

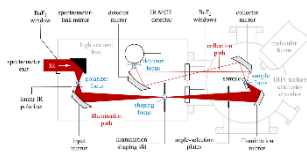
c) DFT - ML Polarons



A team around first author [Viktor Birschtzky](#) leveraged machine learning and a first-principles database to analyze the distribution of surface oxygen vacancies and induced small polarons on rutile  $\text{TiO}_2(110)$  to disentangle the interactions between polarons and defects. Their article “[Machine learning-based prediction of polaron-vacancy patterns on the  \$\text{TiO}\_2\(110\)\$  surface](#)” appeared in *npj Computational Materials*. It is a joint publication between P02 ([Ulrike Diebold](#)) and P07 ([Michele Reticcioli](#), [Cesare Franchini](#)).

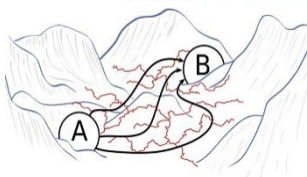


B-site doped perovskite-type oxides were the target of study of [Karin Föttinger's](#) sub-project P10. They published their results in an article entitled “[Cu-doped perovskite-type oxides: A structural deep dive and examination of their exsolution behaviour influenced by B-site doping](#)”, which appeared in *Catalysis Today*. Well done!

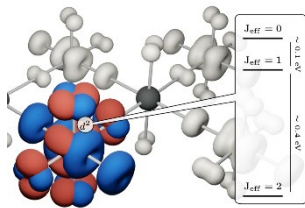


[David Rath](#) et al. present their “[Infrared Reflection Absorption Spectroscopy Setup with Incidence Angle Selection for Surfaces of Non-Metals](#)” in the journal *Review of Scientific Instruments*. While the article still has to appear online in the journal, you can already read it on the [arXiv](#).

Transition Paths ← SPEX → Configurations



A new simulation method that boosts the study of rare yet critical molecular processes was presented by [Sebastian Falkner](#) et al. (P12). The method called SPEX was presented in the article “[Enhanced Sampling of Configuration and Path Space in a Generalized Ensemble by Shooting Point Exchange](#)”, published in *Physical Review Letters*. The University of Vienna highlighted the [achievement](#) on its website. Congratulations!



[Cesare Franchini](#), PI of P07, is the corresponding author of a paper that investigates “[Spin-orbital Jahn-Teller bipolarons](#)”. Two seemingly mutually exclusive interactions are entangled in the material  $\text{Ba}_2\text{Na}_{1-x}\text{Ca}_x\text{OsO}_6$  ( $0 < x < 1$ ). The article was prominently published in [Nature Communications](#).



## 4. New Projects and Grants



No new grants reported.

## 5. Awards and Achievements



[Christoph Schattauer](#), a former postdoc in P02, received his PhD *sub auspiciis Praesidentis rei publicae*. He completed his thesis “Defects in two-dimensional crystals” under the supervision of Prof. Florian Libisch. Congratulations, Christoph!



In April, Harsharan Kaur (P11) received the 2nd poster prize at the European Conference On Non-Linear Optical Spectroscopy (ECONOS) 2024. The conference was co-organized by Ellen Backus, PI of sub-project P11.

## 6. Miscellaneous



Many of you participated actively in the *Lange Nacht der Forschung* (Long Night of Research) on May 24 – thank you so much! It was a great success: The main building of the [University of Vienna](#) counted 3500 visitors, and at [TU Wien](#), we had about 500 visitors in the TUtheSky (though certainly not all at our booths). The front page depicts two group pictures of active TACO participants (and friends). However, the group pictures are not complete: More TACO people than pictured contributed to the success of this great outreach event, in particular Ellen Backus, Moritz Zelenka, and Christoph Dellago. Let's thank them all!



Mira Todorova, MPIE:  
Insights into electrochemical  
solid/liquid interfaces



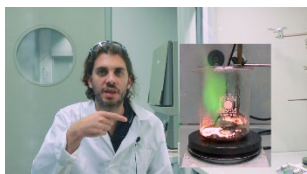
The video of the colloquium talk by [Mira Todorova](#) (MPI for Sustainable Materials) about “[Insights into electrochemical solid/liquid interfaces under potential control from first principles and atomistic calculations](#)” from October 2023 went online recently.



Julia Stähler, HU Berlin:  
How Hybrid Excitons Suppress  
Charge Separation:  
Ultrafast, but Delayed



[Julia Stähler](#) from HU Berlin gave a colloquium talk about “[How hybrid excitons suppress charge separation: ultrafast, but delayed](#)” at the beginning of this summer term. Her talk is also available on our YouTube channel now.



In an informative [short video](#), [Alberto Tampieri](#) from P10 guides us through his lab at the Institute of Materials Chemistry to explain the combustion synthesis of nanocrystalline spinel oxides by burning salts. The video features a few spectacular explosive reactions – enjoy!

Our [YouTube channel](#) is an excellent opportunity to follow inspiring talks even when you missed them or listen to them again. You are welcome to subscribe to the channel and give the videos some thumbs-up! If you are on Twitter, you can follow [our account here](#); if you are on LinkedIn, you will find [the same opportunity here](#).