

**TACO**

TAMING COMPLEXITY  
TOGETHER

**TACO Newsletter**  
**01/2022**



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Reporting period: ~May – July 2022

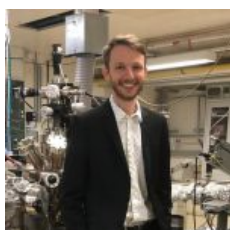
## 1. Personnel Developments



[Christoph Rameshan](#), Co-PI of P10, has been appointed Professor for electrochemical energy conversion and head of the Institute of Physical Chemistry at the Montanuniversität Leoben. He will start his new position in October. Congratulations, Prof. Rameshan!



[Alberto Tampieri](#) started as a new postdoc with Karin Föttinger in subproject P10. Welcome to TACO, Alberto!



[Michael Brunthaler](#) successfully defended his master thesis. He is the first TACO student to graduate. Congratulations and all the best for your future developing new materials for string instruments!

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

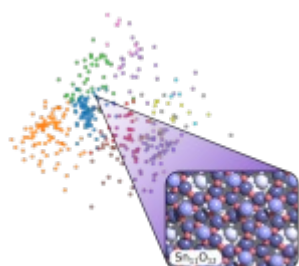
## 2. Upcoming Events



**14. – 16. Sept. 2022:** We will have our first annual TACO Retreat in [Steinschaler Dörfel](#), Frankenfels, in Lower Austria. Be prepared for a real retreat! The scientific program is under construction; it will be sent out soon.

The **TACO colloquia** will be resumed in the new semester. Speakers and dates are currently being fixed. Please keep your schedule free for colloquia on Mondays from around 4 pm onwards!

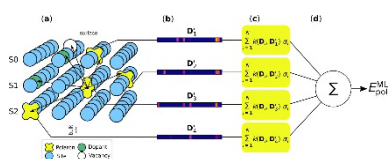
### 3. TACO Papers



An article co-authored by, amongst others, TACO members Michael Schmid and Ulrike Diebold and TACO SAB member Bjørk Hammer about [“Machine-Learning Enhanced Global Optimisation of an Ultrathin Tin Oxide Film Structure”](#) was published in *Angewandte Chemie*. The reviewers ranked the paper in the top 10 % of highly important articles.



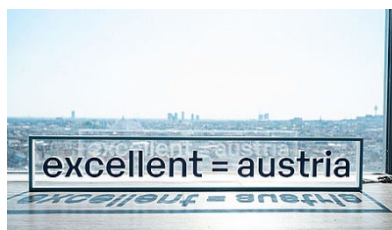
Christoph Rameshan, Co-PI of P10, is co-author of a recently published [Science paper by Peter Amann et al. on methanol synthesis](#). Congratulations!



A team of TACO scientists led by Viktor Birschtzky succeeded in taming complexity in polaron configurational space: They present a new machine-learning approach to accelerate polaron distribution calculation in a [recently published npj Computational Materials article](#).

Your TACO-related article was published recently? Inform the science manager [Stefan Uttenthaler](#) about it!

## 4. New Projects and Grants



The preproposal “Materials for Energy Conversion and Storage (MECS)” for the FWF call “Clusters of Excellence” [made it to the final evaluation stage](#) and was invited to submit a full proposal. Several TACO scientists are involved in this proposal, foremost of all Günther Rupprechter as the Director of Research of the cluster. The deadline for the full proposal submission is October 17.



Gareth Parkinson secured two new projects: First, postdoc Yin Hao will join his group at TU Wien as a Marie Curie Fellow to work on advanced single atom electrochemistry from November. Second, he joins forces with groups in Prague and Ulm in an EU Teaming Grant called NanoCat. This three-year project focuses on studying nanocatalysis by well-defined model systems prepared in UHV conditions.

## 5. Awards and Achievements



[Gareth Parkinson](#), PI of P04, was elected American Vacuum Society Fellow. Congratulations!



Karin Föttinger and her students [developed a new MoS<sub>2</sub> catalyst](#) that can form methanol out of CO<sub>2</sub>. They filed a patent for the process. The new catalyst could make industrial processes more climate-friendly.



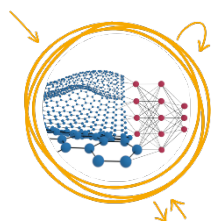
Georg Kresse, TACO Deputy Speaker and PI of P03, received an [honorary doctorate](#) from Lund University (Sweden). Congratulations to Georg!



TACO speaker Ulrike Diebold was [elected vice-president](#) of the Austrian Academy of Sciences. She started the new position on July 1, 2022.



## 6. Miscellaneous



Early reports say that the summer school “Machine Learning for Materials Hard and Soft” was a complete success. Christoph Dellago (Uni Wien), organiser of the school, says: “The Summer School “Machine Learning for Materials Hard and Soft”, which took place July 11-22, 2022, and was organized jointly by the Erwin Schrödinger Institute (ESI) the Doctoral College Advanced Functional Materials (DCAFM) and the Special Research Area TACO, was a great success.

Following a mathematical introduction and a lecture about image analysis, the participants learned about ML for electronic structure, machine-learned force fields, statistical sampling, and materials design in lectures and hands-on tutorials. A particular highlight was the day with research seminars and short talks from the industry. During the two weeks of the school, the participants worked hard, but I think they had a great experience and went home with a lot of new knowledge and inspiration for their own research.” Photos taken at the summer school [support this assessment](#). A more detailed report will be published on the TACO website.



Anna Regoutz, UC London:  
Recent developments in  
Hard X-ray Photoelectron Spectroscopy  
&  
Combination with Theoretical Approaches



TACO Colloquium  
23 May 2022

The most recent [video](#) on the TACO YouTube channel is the colloquium talk about “Recent Developments in Hard X-ray Photoelectron Spectroscopy and Theory” by Anna Regoutz. Please give it some thumbs-up and subscribe to the channel!