

TACO

TAMING COMPLEXITY
TOGETHER

TACO Newsletter
01/2023



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Reporting period: December 2022 – January 2023

1. Personnel Developments



On December 16, 2022, [Philipp Winkler](#) successfully finished his Ph.D. by defending his doctoral thesis “In situ correlative microscopy of hydrogen oxidation on Rhodium-based model catalysts”. Congratulations!

He will continue his research as postdoc in Günther Rupprechter’s project P08.

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

2. Upcoming Events



February 12-15, 2023: The second annual TACO PhD meeting will take place in the JUFA hotel Schladming. Jesús Carrete Montaña, Jiří Pavelec, and Moritz Eder designed the scientific program, which will see invited talks by Barbara Lechner (TU Munich), Gerhard Mestl (Clariant), Livia Bartók-Pártay (University of Warwick), Jennifer Strunk (Leibniz-Institut für Katalyse), Pavel Jelinek (Palacký University, Olomouc, CZ), and Lutz Hammer (Friedrich-Alexander-University of Erlangen-Nürnberg). Last preparations for the meeting are ongoing!

The colloquia in the summer term of 2023 will retake place at TU Wien. [Kristian Sommer Thygesen](#) will give a colloquium talk on April 17. Further preparations are underway.

The highlight of the year will be our conference **“Taming Complexity in Materials (TACO): Synergies between Experiment and Modeling”**, which will take place at TUtheSky from September 24-27. Mark your calendars! Confirmed invited speakers are: Bilge Yildiz (MIT), Boris Kozinsky (Harvard University), Beatriz Roldan (FHI Berlin), Karsten Reuter (FHI Berlin), Frank Noe (FU Berlin), Martin Setvin (Charles University Prague), Ralf Drautz (Ruhr University Bochum), Tanja Cuk (University of Colorado, Boulder), Johannes Kästner (University of Stuttgart), and Zdenek Dohnalek (PNNL).

3. TACO Papers

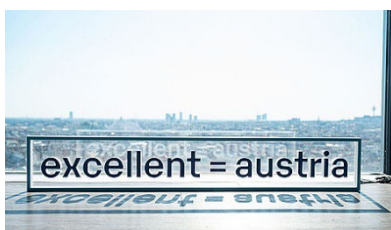


No new publication since the last issue of the TACO Newsletter? This cannot be. Most probably, you haven't told the science manager [Stefan Uttenthaler](#) about your outstanding scientific work!

4. New Projects and Grants



We congratulate [Andreas Grüneis](#) for receiving an ERC Consolidator Grant! He will use the grant to develop methods of quantum physics to calculate material properties from first principles. Many TACO scientists know Andreas well, and his computational methods such as coupled-cluster theory should be interesting for TACO people.



The proposal “Materials for Energy Conversion and Storage (MECS)” for a Clusters of Excellence will enter the decisive phase with a hearing in front of the international jury soon after the TACO PhD meeting. Several TACO PIs are involved in this large project. The Austrian Science Fund FWF will communicate the decision in early March.

5. Awards and Achievements



No prize was awarded in the reporting period.

6. Miscellaneous



Nuria Lopez, ICIQ Barcelona:
Dynamic Metal Charge States
in Single Atom Catalysis



TACO Colloquium
28 November 2022

We have new videos of TACO Colloquia talks on our YouTube channel. Nuria Lopez (Institute of Chemical Research of Catalonia) spoke about [Dynamic Metal Charge States in Single Atom Catalysis](#) in November.



Alessandro Fortunelli, CNR Pisa:
Mechanisms of the Oxygen Evolution Reaction
on NiFe₂O₄ and CoFe₂O₄ Inverse-Spinel Oxides



TACO Colloquium
12 December 2022

Alessandro Fortunelli (CNR Pisa) presented [Mechanisms of the Oxygen Evolution Reaction on NiFe₂O₄ and CoFe₂O₄ Inverse-Spinel Oxides](#).

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! Just follow the links above.

If you are on Twitter, you can follow [our account here](#); if you are on LinkedIn, you will find [the same opportunity here](#).