

TACO Newsletter

01/2024



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Reporting period: December 2023 – January 2024

1. Personnel Developments



[Camilla Ferreira de Sá Codeço](#) is a new visiting professor in the group of Günther Rupprechter (P08).



Congratulations to [Lukas Bogner](#)! He finished his master's thesis in the group of Ellen Backus (P11). Lukas will continue pursuing a Ph.D. in Ellen's group but not related to TACO.



The same congratulations go to [Florian Dörr](#)! He finished his master's thesis in the group of Ulrike Diebold (P02). Florian will continue as a Ph.D. student to work on ViPeRLEED

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

2. Upcoming Events



The TACO Ph.D. Meeting will happen in Schladming from February 11-14, 2024. The SOC, composed of [Johannes Zeininger](#) (P08), [Ralf Wanzenböck](#) (P09), [Alberto Tampieri](#) (P10), and [Harsharan Kaur](#) (P11), successfully attracted the following invited speakers:

[Liliana Lukashuk](#) (Johnson Matthey), [Marc Georg Willinger](#) (TU Munich), [Davide Ferri](#) (Paul Scherrer Institute), [Markus Valtiner](#) (TU Wien), and [Zachary Ulissi](#) (Meta & Carnegie Mellon University, online).

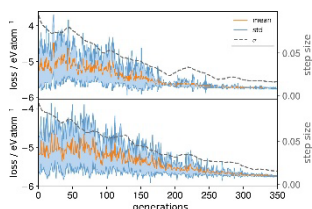
The [program](#) is online on our website.

The following talks in the TA[CO]lloquium series in the summer term of 2024 have been arranged:

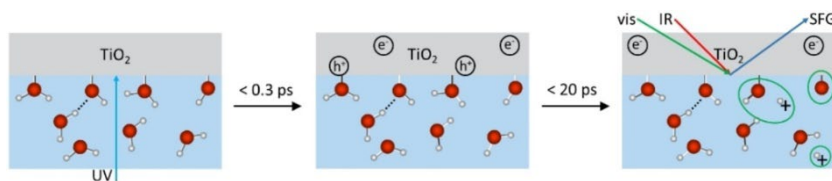
Date	Speaker	Title
March 04	Julia Stähler (HU Berlin)	<i>Right on Time: Ultrafast Charge Separation before Hybrid Exciton Formation</i>
April 15	Mariana Rossi (MPI Hamburg)	<i>Weakly Bound Materials: Competing Energy Scales, Quantum Effects, and Machine Learning</i>
May 13	Daniel Boese (Uni Graz)	<i>Intermolecular Interactions: Surfaces, Molecules, and Molecular Crystals</i>

The talks will take place at TU Wien again. **Attention: The talk on March 4 will occur in a new place, namely in the lecture room on the 5th floor of the main library of TU Wien (the building with the owls).** There will be no colloquium in June because we will need the time to write the report and the TACO renewal proposal!

3. TACO Papers



A new paper is coming from subproject P09 ([Georg Madsen](#)) with first-author [Ralf Wanzenböck](#). Their article "[Clinamen2: Functional-style evolutionary optimization in Python for atomistic structure searches](#)" describes a versatile functional-style Python implementation of the covariance matrix adaptation evolution strategy (CMA-ES) called Clinamen2 that enables atomistic structure searches. The article appeared in *Computer Physics Communications*. Congratulations!



[Ellen Backus](#) and [Moritz Zelenka](#) of subproject P11, together with other authors, used femtosecond time-resolved, surface-specific vibrational sum frequency generation spectroscopy to study at the molecular level the photo-induced water dissociation at the interface of TiO_2 with liquid water. They published their results in the article "[Ultrafast Surface-Specific Spectroscopy of Water at a Photoexcited \$\text{TiO}_2\$ Model Water-Splitting Photocatalyst](#)" in *Angewandte Chemie*. Well done!

Did you publish a paper in the framework of TACO? Inform the science manager [Stefan Uttenthaler](#)!

4. New Projects and Grants



Great succes for [Matthias Meier](#)! His stand-alone grant proposal to the FWF entitled "[Advances in Single-Atom-Polaron Catalysis](#)" was approved in the board meeting in November. In this project, Matthias will improve a computational framework to study the effect of polarons on the surface properties and their interaction with single atoms and their catalytic properties. He will carry out the project at the University of Vienna. Congratulations to Matthias!

5. Awards and Achievements



We proudly announce a great success from [Karin Föttinger](#) and her group (P10)! Her project "[co2ol catalyst](#)" (speak: "cool catalyst") is one of three greenstar(t) [award-winning projects](#) that received a 20,000 € prize from the climate ministry to boost climate-relevant ideas. The "co2ol catalysts" project seeks to develop catalysts that make methanol out of industry CO₂ emissions for further processing. The funds will be used to support a start-up company to develop the catalysts for the industry further. Congratulations, Karin!



[Alberto Tampieri](#), post-doc in the same subproject P10, was awarded a "[Premis Extraordinaris de Doctorat](#)" for his doctoral thesis conducted at the Universitat Rovira i Virgili (Tarragona, Spain). Congratulations, Alberto!



[Günther Ruppachter](#), PI of subproject P08, became a member of the European Academy of Sciences, as TU Wien [reported on LinkedIn](#). Congratulations, Günther!



From the same subproject P08, the *Nature Communications* article "[Lanthanum modulated reaction pacemakers on a single catalytic nanoparticle](#)" by [Maximilian Raab](#) et al. was highlighted by a [press release](#) on the TU Wien website. Well done!

6. Miscellaneous



The TA[CO]lloquium talk by Edvin Lundgren about "[*Surface-Sensitive Studies of the Electrolyte-Electrode Interface*](#)" was recorded and you can watch it on our YouTube channel!

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](#).