

# **TACO Newsletter**

## **04/2024**



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Reporting period: June – July 2024

## 1. Personnel Developments



Many new people joined our group ahead of the submission deadline of the TACO renewal proposal. No new people joined in the reporting period. In case new people join your subproject, please inform the science manager [Stefan Uttenthaler](#)!

## 2. Upcoming Events



The **TACO Retreat** will take place on **September 23-25** in Steinschaler Dörfel, Frankenfels, Lower Austria. We will have the following top-notch invited speakers, for most of which we already know the title:

[Gregory S. Rohrer](#) (Carnegie Mellon University): “Modifying SrTiO<sub>3</sub> Surfaces to Maximize Photochemical Water Splitting”

[Alexandre Tkatchenko](#) (University of Luxemburg): “Towards AI-enabled Fully Quantum (Bio)Molecular Simulations”

[Marta Gibert](#) (TU Wien): “Atomically-Engineered Magnetic Double-Perovskite Oxide Heterostructures”

[Paul A. Fenter](#) (Argonne National Laboratory): “Unexpected Complexity in the Reactivity of Solid-Water Interfaces”

[Kieron Burke](#) (UC Irvine): Title tba

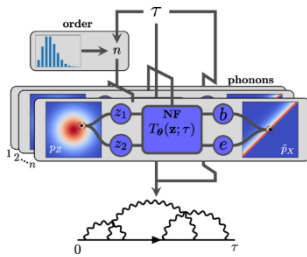
We will also use the retreat to prepare for the **FWF hearing** in the framework of the TACO interim evaluation. The hearing will take place on **Thursday, October 17**.

The **TACO PhD Meeting 2025** will be held from **February 2 to 5** in Sporthotel Royer.

The current **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 (rooms tba). We plan to have an additional talk in December; a request is ongoing.

<b>Date</b>	<b>Speaker</b>	<b>Title</b>
November 11	<a href="#">Xavier Gonze</a> (UC Louvain, Belgium)	<i>tbd</i>
January 13	<a href="#">Sereina Riniker</a> (ETH Zurich, Switzerland)	<i>tbd</i>
January 27	<a href="#">Karsten Reuter</a> (Fritz Haber Institute, Germany)	<i>tbd</i>

### 3. TACO Papers



Luca Leoni and [Cesare Franchini](#) published their paper “[Global sampling of Feynman's diagrams through normalizing flow](#)” in the journal *Physical Review Research*. The authors explore the integration of normalizing flows in the diagrammatic Monte Carlo method, presenting an architecture designed to sample the intricate multidimensional space of Feynman's diagrams through dimensionality reduction. Well done!

## 4. New Projects and Grants



[Esther Heid](#), Co-PI in sub-project P09, was awarded a 1.2 M€ FWF START grant for her project “[Deep learning of chemical reactions](#)”. The project aims to develop new machine-learning algorithms that will allow researchers to find new chemical reactions and catalysts in a computer-based virtual laboratory and accelerate the search for sustainable approaches in chemistry. You can read more about the project on the [website of the FWF](#) or the [TU Wien](#). Congratulations, Esther!

## 5. Awards and Achievements



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– ICC 2024

Ulrike Diebold gave two plenary talks, one at the Condensed Matter and Quantum Materials (CMQM) Conference, St Andrews, Scotland, and a second one at the 8<sup>th</sup> International Congress on Catalysis (ICC18) in Lyon, France.



## 6. Miscellaneous



Mariana Rossi, MPI SD:

Weakly Bound Materials:  
Competing Energy Scales,  
Quantum Effects,  
and Machine Learning



TACO Colloquium  
15 April 2024

The video of the excellent colloquium talk by [Mariana Rossi](#) (MPI for the Structure and Dynamics of Matter) about “[Weakly Bound Materials: Competing Energy Scales, Quantum Effects, & Machine Learning](#)” is available on our YouTube channel now.

Our [YouTube channel](#) is an excellent opportunity to follow inspiring talks 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](#).