

lädt ein

gemeinsam mit der Gesellschaft
Deutscher Chemiker
zum

Vortrag

von Frau

**Prof. Renana
Gershoni-Poranne**

*Technion – Israel
Institute of
Technology/IL*



**“Mission ImPASsible:
Decoding Polycyclic
Aromatic Systems with
Deep Learning”**

am: **Montag, 20.10.2025**

um: **17:15 Uhr**

WO: im Raum **A12.153**

Gäste sind herzlich willkommen!



TECHNISCHE UNIVERSITÄT
IN DER KULTURHAUPTSTADT EUROPAS
CHEMNITZ

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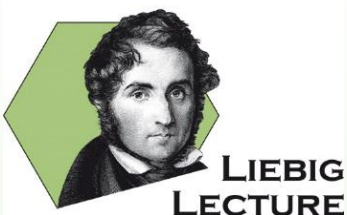


Mission ImPASsible: Decoding Polycyclic Aromatic Systems with Deep Learning

Polycyclic aromatic systems (PASs) present a seemingly insurmountable challenge: vast chemical spaces, complex electronic structures, and elusive aromatic properties. Our mission, should we choose to accept it, is to harness the power of deep learning to decode these molecular mysteries. In this talk, we embark on a journey through this complex chemical space, combining traditional computational methods with cutting-edge artificial intelligence tools. We demonstrate how neural networks can be trained to predict electronic properties with unprecedented speed and accuracy. More importantly, we show how they can be used interpretably to extract chemical insight. This talk will not self-destruct in five seconds, but it will revolutionize how we think about combining artificial intelligence with molecular science.

- [1] The COMPAS Project: *J. Chem. Inf. Model.* **2022**, 62, 3704; *Sci. Data* **2024**, 11, 97; *Beilstein J. Org. Chem.* **2024**, 20, 1817–1830. *Phys. Chem. Chem. Phys.* **2024**, 26, 15344–15357; *J. Chem. Inf. Mod.* **2025**, 65, 5508–5517.
- [2] ML and DL: *J. Phys. Org. Chem.* **2022**, e4458; *J. Org. Chem.* **2023**, 88, 9645–9656; *Nat. Comput. Sci.* **2023**, 3, 873–882.





LIEBIG LECTURESHIP

der Liebig-Vereinigung für Organische Chemie
in der Gesellschaft Deutscher Chemiker

October 2025

Prof. Renana Gershoni-Poranne

Technion – Israel Institute of Technology/IL



Mission ImPASsible: Decoding Polycyclic Aromatic Systems with Deep Learning

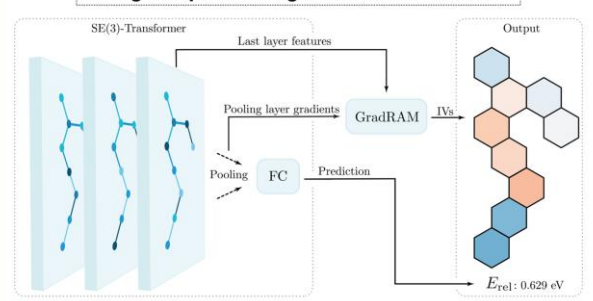
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The COMPAS Project – A dedicated database for PASs



Using Deep Learning to Understand PASs



Freiburg

Monday

October 13th

Gießen

Tuesday

October 14th

Münster

Wednesday

October 15th

Mülheim

Thursday

October 16th

Chemnitz

Monday

October 20th

Regensburg

Tuesday

October 21st

München

Wednesday

October 22nd

Renana Gershoni-Poranne is an Associate Professor in the Schulich Faculty of Chemistry at the Technion, where her group combines quantum chemical calculations, cheminformatics, and machine learning to understand and predict properties and reactivity in organic chemistry, with a particular focus on polycyclic aromatic systems. She received her MSc and PhD from the Technion (Prof. Amnon Stanger, 2015) and then carried out postdoctoral research at ETH Zurich (Prof. Peter Chen). She began her independent career as a Senior Scientist at ETH Zurich and was appointed Assistant Professor at the Technion in 2021.