LIEBIG LECTURESHIP

der Liebig-Vereinigung für Organische Chemie

in der Gesellschaft Deutscher Chemiker

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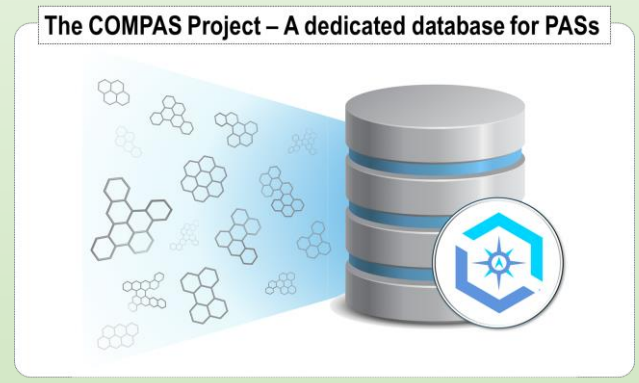
Technion – Israel Institute of Technology/IL

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.

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.