NICOLAUS COPERNICUS
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Faculty of Chemistry

Faculty of Chemistry Nicolaus Copernicus University in Toruń

is pleased to invite to a

faculty seminar

entilted

Beyond DFT: how AI is reshaping organic chemistry simulation

which will be given by

prof. Pavlo Dral

PCOSS, FTCC, College of Chemistry and Chemical Engineering, Xiamen University, China
Institute of Physics, Faculty of Physics, Astronomy, and Informatics, Nicolaus Copernicus University in Toruń, Poland

11.02.2025 at 10:00 am

in our Library

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Abstract

I will present our work on AI to accelerate and improve the accuracy of organic chemistry simulations at the quantum chemical level. This allowed us to discover new chemical phenomena such as roaming in Diels–Alder reaction, where the diene is orbiting around the fullerene C_{60}.[1] In addition, we could revise the understanding of the bifurcating pericyclic reaction mechanism, which we show is stepwise instead of concerted as believed previously.[2] We also reveal the role of the near-lying Cope-rearrangement transition state on the outcome of the bifurcating pericyclic reaction. In addition, we corrected experimental geometries and thermochemical measurements with our out-of-the-box methods. The power of our AI methods extends to uncovering interesting phenomena in the photochemical organic reactions too, such as long-time oscillating behavior in the cis-trans photoisomerization of azobenzene.[3] All of these developments are enabled by the range of our AI methods,[4-5] most of which can make predictions faster and more accurately than popular DFT approaches such as B3LYP/6-31G*. They are accessible to the research community via our open-source software package MLatom[6] and online cloud computing platform.

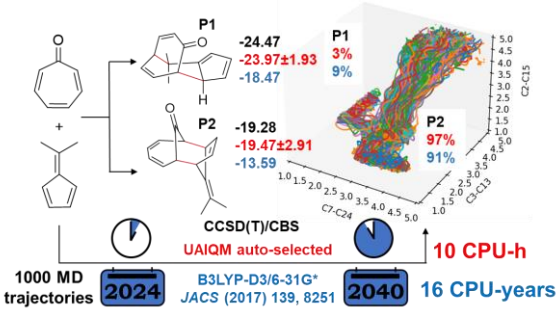

Figure 1. Our AI methods can provide faster and more accurate predictions than standard DFT.[7]

[1] Y. F. Hou, Q. Zhang, P. O. Dral. Surprising dynamics phenomena in Diels–Alder reaction of C_{60} uncovered with AI. *J. Org. Chem.* **2024,** *89*, 15041–15047.
[2] Y. Chen, P. O. Dral. AIQM2: Better Reaction Simulations with the 2nd Generation of General-Purpose AI-enhanced Quantum Mechanical Method. *ChemRxiv. Submission date: 2024-10-08.* **2024.**
[3] M. Martyka, L. Zhang, F. Ge, Y.-F. Hou, J. Jankowska, M. Barbatti, P. O. Dral. Charting electronic-state manifolds across molecules with multi-state learning and gap-driven dynamics via efficient and robust active learning. *ChemRxiv*, *https://doi.org/10.26434/chemrxiv-2024-dtc1w* **2024.**
[4] P. Zheng, R. Zubatyuk, W. Wu, O. Isayev, P. O. Dral. Artificial Intelligence-Enhanced Quantum Chemical Method with Broad Applicability. *Nat. Commun.* **2021,** *12*, 7022.
[5] Y. Rui, Y. Chen, E. Ivanova, V. B. Kumar, S. Smiga, I. Grabowski, P. O. Dral. The Best DFT Functional Is the Ensemble of Functionals. *Adv. Sci.* **2024,** *11*, 2408239.
[6] P. O. Dral, et al. MLatom 3: A Platform for Machine Learning-Enhanced Computational Chemistry Simulations and Workflows. *J. Chem. Theory Comput.* **2024,** *20*, 1193–1213.
[7] Y. Chen, Y.-F. Hou, O. Isayev, P. O. Dral. Universal and Updatable Artificial Intelligence-Enhanced Quantum Chemical Foundational Models. *ChemRxiv. Submission date: 2024-06-26.* **2024.**