Dear All

Professor Pavlo Dral Dr. Pavlo O. Dral (Department of Chemistry, Xiamen University, China, Instytut Fizyki, UMK Toruń)
<http://dr-dral.com> | <http://MLatom.com> (Atomistic Machine Learning) @ <http://XACScloud.com> (Xiamen Atomistic Computing Suite)
<https://xacs.xmu.edu.cn/>,
our expert on AI and ML, will conduct a **10-hour** course entitled **"AI for molecular physics and chemistry simulations"**The course is intended for students, PhD students and  employees.

The participants are expected to have a background knowledge of quantum chemistry and molecular simulations. The knowledge of Python is a plus but not required, however, advanced users might want to install mlatom on their computers before the lectures. No preliminary knowledge of ML is necessary.
The course will take place in the **second half of Januar**y at the Institute of Physics of Nicolaus Copernicus University in Toruń  (the room will be announced later).
There are five meetings of 2 hours each  **18.00-20.00 , January 16, 21, 23, 28, 30  2025**
**Tuesdays: January 21, 28 , 2025
Thursdays: January 16, 23, 30  , 2025**

abstract:

The course "AI for molecular physics and chemistry simulations" teaches essential skills in applying AI for molecular simulations at the quantum chemical levels. It consists of plenty of hands-on exercises going along with the fundamental theoretical background. The course will introduce the state of the art machine-learning (ML) approaches for accelerating and improving accuracy of quantum chemical simulations. It will also use the established program for such simulations, MLatom, providing an excellent tool set for both complete beginners and advanced students. At the end of the course, the students will be able to create their own ML interatomic potentials and custom models, run ML simulations including ground- and excited-state molecular dynamics, various types of spectroscopy (IR, Raman, UV/vis, two-photon absorption), explore reaction mechanisms, and build their own data sets via active learning approaches.

Due to the limited number of places, all interested in participating in the course are asked to **register with Ms. Joanna Kozłowska** **<joanna.kozlowska@umk.pl>** **by January 9, 2025.**In addition to practical knowledge, participants will receive a certificate confirming the completion of the course