Towards practical AI-enhanced computational chemistry

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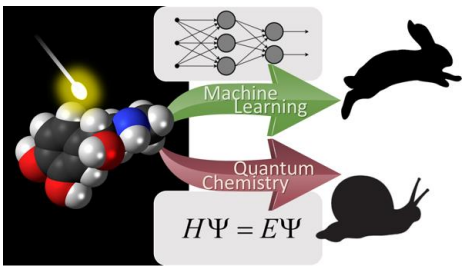

Machine learning greatly speeds up quantum mechanical simulations.[1]

I will present our methods and software tools enabling practical AI-enhanced computational chemistry simulations and demonstrate their applications. The methods include the general-purpose, artificial intelligence-enhanced quantum mechanical method 1 (AIQM1),[2] which approaches the accuracy of golden-standard, traditional CCSD(T)/CBS approach for many properties. Other methods focus on novel approaches for learning dynamics such as our AI-quantum dynamics [3] and 4D-spacetime atomistic AI[4] approaches which predict dynamics properties such as nuclear coordinates as the function of time and do not require iterative trajectory propagation as in classical MD. AIQM1 and AI-QD along with many other methods such as a host of ML interatomic potentials are implemented in our MLatom program package and Python library for user-friendly atomistic machine learning simulations which can be run online using our MLatom@XACS (Xiamen atomistic computing suite) cloud-based service.[5]

[1] P. O. Dral, M. Barbatti. Molecular Excited States Through a Machine Learning Lens. *Nat. Rev. Chem.* **2021,** *5*, 388–405.

[2] 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.

[3] A. Ullah, P. O. Dral. Predicting the future of excitation energy transfer in light-harvesting complex with artificial intelligence-based quantum dynamics. *Nat. Commun.* **2022,** *13*, 1930.

[4] F. Ge, L. Zhang, Y.-F. Hou, Y. Chen, A. Ullah, P. O. Dral. Four-Dimensional-Spacetime Atomistic Artificial Intelligence Models. *J. Phys. Chem. Lett.* **2023,** *14*, 7732–7743.

[5] a) P. O. Dral, F. Ge, B.-X. Xue, Y.-F. Hou, M. Pinheiro Jr, J. Huang, M. Barbatti. MLatom 2: An Integrative Platform for Atomistic Machine Learning. *Top. Curr. Chem.* **2021,** *379*, 27. b) P. O. Dral, F. Ge, Y.-F. Hou, P. Zheng, Y. Chen, M. Barbatti, O. Isayev, C. Wang, B.-X. Xue, M. Pinheiro Jr, Y. Su, Y. Dai, Y. Chen, S. Zhang, L. Zhang, A. Ullah, Q. Zhang, Y. Ou. MLatom 3: Platform for machine learning-enhanced computational chemistry simulations and workflows. *arXiv:2310.20155v1 [physics.chem-ph]* **2023**.See MLatom.com @ XACScloud.com.

Biography

Pavlo O. Dral is a Full Professor and an Assistant Dean in international admissions matters at the Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University. His research is focused on AI for quantum chemistry and dynamics. Pavlo O. Dral is a founder of the *MLatom* package for atomistic machine learning simulations and a co-founder of the *Xiamen Atomistic Computing Suite*. He is an Editor of the journals *Artificial Intelligence Chemistry* and *SciPost Chemistry*. Pavlo O. Dral is the author of ca. 60 peer-reviewed articles including publications in *Nat. Comm.*, *Adv. Sci.*, and *Nat. Rev. Chem.* as well as 10 book chapters, and the editor of the book on AI for quantum chemistry. His h-index is 25 with ca. 4500 citations. In 2021, Pavlo O. Dral was awarded an Outstanding Youth (Overseas) by the National Natural Science Foundation of China. More information is available on Dral's group website dr-dral.com.