Accelerating and improving quantum chemistry and dynamics with artificial intelligence

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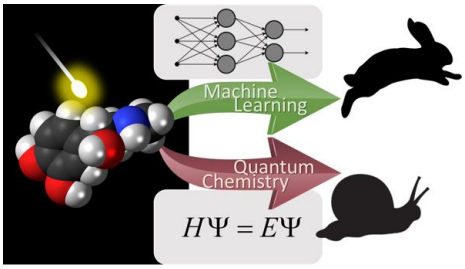

Machine learning greatly speeds up quantum mechanical simulations.[1]

I will present our recent developments in applying artificial intelligence to enhance quantum chemistry and (quantum) molecular dynamics simulations. One of these developments is general-purpose, artificial intelligence-enhanced quantum mechanical method 1 (AIQM1),[2] which approaches the accuracy of golden-standard, traditional CCSD(T)/CBS approach for closed-shell, neutral organic molecules in their ground state at the speed of semiempirical quantum mechanical methods while retaining good accuracy for charged systems and excited states. This method does not need retraining and enables us to perform simulations we have not been able to do with either traditional quantum chemical approaches or with experimental techniques. Another development is our artificial intelligence-based quantum dynamics (AI-QD) approach which does not require iterative trajectory propagation.[3] Finally, I will talk about creating atomistic artificial intelligence models in 4D spacetime as an efficient tool for investigating molecular dynamics.[4] AIQM1 and AI-QD along with many other methods are implemented in our *MLatom* program package 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, A. Ullah, P. O. Dral. Four-dimensional spacetime atomistic artificial intelligence models. **2022,** preprint on ChemRxiv: http://doi.org/10.26434/chemrxiv-2022-qf75v

[5] 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. See http://mlatom.com @ http://xacs.xmu.edu.cn.