Machine Learning-Assisted Fully Quantum (Bio)Molecular Simulations : From Dream to Reality

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Abstract

The convergence between accurate quantum-mechanical (QM) models (and codes) with efficient machine learning (ML) methods seem to promise a paradigm shift in molecular simulations. Many challenging applications are now being tackled by increasingly powerful QM/ML methodologies. These include modeling covalent materials, molecules, molecular crystals, surfaces, and even whole proteins in explicit water (https://www.science.org/doi/abs/10.1126/sciadv.adn4397). In this talk, I attempt to provide a reality check on these recent advances and on the developments required to enable fully quantum dynamics of complex functional (bio)molecular systems. Multiple challenges are highlighted that should keep theorists in business for the foreseeable future:

(1) Ensuring the accuracy of high-level QM methods (https://doi.org/10.1038/s41467-021-24119-3; https://doi.org/10.1038/s41586-023-06587-3),
(2) Describing intricate QM long-range interactions (https://doi.org/10.1126/sciadv.aax0024; https://doi.org/10.1126/science.aae0509; https://doi.org/10.1103/PhysRevLett.128.106101),
(3) Treating quantum electrodynamic effects that become relevant for complex molecules (https://doi.org/10.1021/acs.jpclett.1c04222; https://doi.org/10.1103/PhysRevResearch.4.013011).
(4) Developing increasingly accurate, efficient, scalable, and transferable ML architectures for molecules and materials (https://doi.org/10.1038/s41467-022-31093-x; https://arxiv.org/abs/2209.14865; https://arxiv.org/abs/2209.03985).
(5) Accounting for the quantum nature of the nuclei and the influence of external environments (https://doi.org/10.1038/s41467-020-20212-1; https://doi.org/10.1038/s41467-022-28461-y).

I argue that only a conjunction of all these developments will enable the long-held dream of fully quantum (bio)molecular simulations.

-About the speaker

Alexandre Tkatchenko is a professor and head of the Department of Physics and Materials Science at the University of Luxembourg, where he holds a chair in Theoretical Chemical Physics. Tkatchenko also holds a distinguished visiting professor position at the Technical University of Berlin and has co-founded two deeptech startups. His group develops accurate and efficient first-principles computational models to study a wide range of complex materials, aiming at qualitative understanding and quantitative prediction of their structural, cohesive, electronic, and optical properties at the atomic scale and beyond. He has delivered more than 400 invited talks, seminars and colloquia worldwide, published ~220 articles in prestigious journals (h-index of 84 with more than 41,000 citations; Top 1% ISI highly cited researcher in 2018-2023), and serves on the editorial boards of four society journals: Science Advances (AAAS), Physical Review Letters (APS), Chemical Science (RSC), and the Journal of Physical Chemistry Letters (ACS). Tkatchenko has received a number of awards, including APS Fellow from the American Physical Society, Fellow of

the Royal Society of Chemistry (FRSC), Gerhard Ertl Young Investigator Award of the German Physical Society, Dirac Medal from the World Association of Theoretical and Computational Chemists (WATOC), Feynman prize from the Foresight Institute, van der Waals prize of the international conference on non-covalent interactions (ICNI), and five flagship grants from the European Research Council: a Starting Grant in 2011, a Consolidator Grant in 2017, an Advanced Grant in 2022, and Proof-of-Concept Grants in 2020 and 2023.