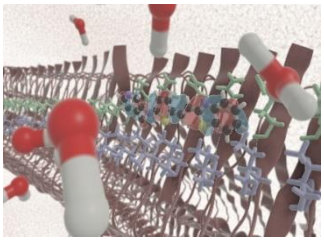
VeloxChem: Science and education-enabling platform for quantum molecular modeling

PATRICK NORMAN, MATHIEU LINARES

[a]*Division of Theoretical Chemistry and Biology, KTH Royal Institute of Technology*
[b]*PDC Center of High Performance Computing, KTH Royal Institute of Technology*



VeloxChem[1] is a science- and educational-enabling software platform for quantum molecular modeling at the levels of DFT and TDDFT. It is strictly object-oriented and written in a hybrid of the Python and C++/CUDA/HIP programming languages and it implements extremely efficient parallelism through MPI and OpenMP. Noteworthy functionalities include real and complex response functions up to cubic order with geometric derivatives of complex linear response functions to enable resonance Raman spectrum simulations and built-in interoperability with classical molecular dynamics simulations by means of an automatized force-field generation. It installs with conda on Windows/macOS/Linux personal computers as well as it can harness the power of modern supercomputers with GPU hardware acceleration.

Largely based on VeloxChem is the eChem[2] Jupyter book initiative that allows for interactive deep learning of the theory and methods in theoretical chemistry. The Jupyter notebooks upon which this electronic book is built present theory and numerical methods with intertwined illustrative Python code cells. In addition to this educational aspect, we find notebooks to be useful for code prototyping as a means to accelerate the process of software development.

The VIAMD graphical user interface enables visual interactive analysis of the complex[3] molecular systems that VeloxChem can address, including the electronic structures of ground and excited states together with the associated transition densities.

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[1] Rinkevicius, Z.; Li, X.; Vahtras, O.; Ahmadzadeh, K.; Brand, M.; Ringholm, M.; List, N. H.; Scheurer, M.; Scott, M.; Dreuw, A.; Norman, P. VeloxChem: A Python-driven Density-functional Theory Program for Spectroscopy Simulations in High-performance Computing Environments. *WIREs Comput Mol Sci* **2020**, *10* (5), e1457.

[2] Fransson, T.; Delcey, M. G.; Brumboiu, I. E.; Hodecker, M.; Li, X.; Rinkevicius, Z.; Dreuw, A.; Rhee, Y. M.; Norman, P. eChem: A Notebook Exploration of Quantum Chemistry. *J. Chem. Educ.* **2023**, *100* (4), 1664–1671.

[3] R Skånberg, I Hotz, A Ynnerman, M Linares, VIAMD: a Software for Visual Interactive Analysis of 3 Molecular Dynamics, J. Chem. Inf. Model. **2023**, 63, 23, 7382–7391.