Molecular Properties and Theoretical Spectroscopy Simulations in HPC Cluster Environments with VeloxChem

I. E. Brumboiu[1], P. Norman[2]

[1] *Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, 87-100 Toruń, Poland*
[2] *Division of Theoretical Chemistry and Biology, KTH Royal Institute of Technology, 100 44 Stockholm, Sweden*

iubr@umk.pl

Here we present software development efforts for efficient molecular properties and theoretical spectroscopy simulations of very large molecular systems (up to and beyond 500 second row atoms), either free-standing or in the presence of an environment. These developments are carried out in VeloxChem [1], an MPI/OpenMP parallel Python-driven quantum chemistry software suitable for high-performance computing (HPC) cluster environments. VeloxChem implements an efficient multifrequency complex linear response equation solver which enables calculations of core and valence electronic absorption and circular dichroism spectra, as well as a quadratic response solver which can be used to determine observables related to second-harmonic generation (SHG) [2] at the Hartree–Fock and Kohn–Sham Density Functional Theory (DFT) levels. Besides its HPC aspects, VeloxChem also features interactive program access through Jupyter notebooks which makes it an education-enabling software platform for quantum molecular modeling, as illustrated in the eChem project [3]. Here, we will focus on the HPC aspects of VeloxChem and illustrate its performance for various spectroscopies and molecular properties of very large systems. One particular example will be related to the valence electronic structure of a hydrogen-bonded layer of melamine deposited on a Au(111) surface. We will illustrate the effects of hydrogen bonding on the valence unoccupied electronic states of melamine as determined with Near-edge X-ray absorption fine structure (NEXAFS) spectroscopy.

[1] Rinkevicius, Zilvinas *et al*., WIREs: Comput. Mol. Sci., **10**, e1457 (2020)
[2] Ahmadzadeh, Karan *et al*., *Electron. Struct.,* **4**, 044004 (2022)
[3] Fransson, Thomas *et al.*, *J. Chem. Educ.*, **100**, 1664–1671 (2023)