Prediction of properties for sizable molecular systems including spin-orbit effects

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We will present our efforts to expand the usability of the quasirelativistic two-component (2c) GW/(c)BSE and hybrid time-dependent(TD)-DFT methods to calculate properties of large molecules containing heavy elements [1]. For the properties of these compounds spin-orbit effect can often not be neglected if a quantitative description is sought for. To efficiently obtain results from GW/(c)BSE [2] highly optimized 2c contour-deformation (CD) and analytic-continuation (AC) GW methods within the resolution-of-the-identity approximation (RI) are used, allowing us to compute properties for sizable systems at local compute nodes also for extended sets of molecules. For 2c hybrid TD-DFT RI-K and seminumerical algorithms for exchange were implemented, allowing to obtain spin-orbit dependent properties of molecules with hundreds of atoms. Further the two-component extension of the current-dependent metaGGA response [3] formalism was implemented. This is crucial to describe antiferromagnetic coupled systems or current-carrying states, where the current is induced by spin-orbit coupling itself or external fields, e.g. magnetic fields. Finally, a tool converting theoretical and experimental spectra to common variables known by workers in both fields (e.g. RGB colour codes) was implemented within the TURBOMOLE program package to allow for a rapid comparison between experimental and theoretical data. Due to the combined efficiency and robustness of the developed algorithms many possible molecular candidates containing heavy elements can be screened on locally available compute nodes, e.g. helping to identify the molecular structure of compounds where other standard methods as X-ray crystallography cannot readily be used.
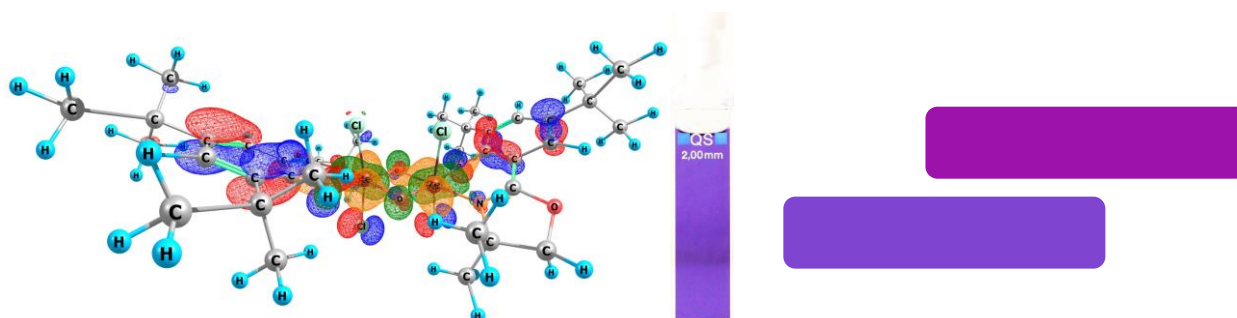

Figure 1: left: trial molecule, middle: picture of measured sample, upper right: calculated color (2c GW/cBSE@PBE0) from a possible trial compound, lower right: measured color from sample compound.

References
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