An Infrastructure for Processing Quantum Chemical Data:

Illustrations in the Context of Molecular Design and Method Development

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The computational infrastructure (hard- and software) available to quantum chemists has grown enormously, making increasingly complex systems feasible for accurate computation. Since the generation of the data (results) is no longer the bottleneck, the challenge now is to find strategies for structured storage, extraction (analysis) and interchange of data, thereby keeping the level of human intervention at a minimum.

Here we report on the implementation of a workflow scheme using TURBOMOLE as application program package, an extension of CML as interchangeable output format, as well as FoXlib and eXist to write out and store the data.

To illustrate the benefit of structured data processing, we present the results of an extensive study on the stability of the RI-MP2-F12 method with respect to combinations of auxiliary basis sets used. The test set consists of a small array of conformers of the ethene dimer invoking more than 5'000 computations. Furthermore, using advanced analysis and data processing, we will show that the impact of a donor- or acceptor-substituent attached to a π-conjugated backbone will decay according to an exponential law.