

Automation of computational chemistry and machine learning workflows

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Continued improvements in computer hardware and algorithms have allowed quantum chemical methods to be employed for studying more complex and larger molecules. However, performing the various computational protocols required for high-throughput screening, molecular optimization, and machine learning (ML) model training can be tedious and time-consuming. For example, a sequence of molecule building, conformational sampling, geometry optimization, thermochemical analysis, property prediction, and ensemble averaging is often performed. Each step may involve a different model chemistry executed by a separate package. Automating these workflows minimizes errors, enhances reproducibility, and facilitates storing and reusing the associated data.

Automated workflows for quantum mechanical (QM) calculations, including those that address the important challenge of transition state (TS) location and conformational analysis, have emerged as powerful software tools. In this talk, we present AQME, [1] an automated end-to-end workflow software that performs multi-step tasks of computational chemistry, and ROBERT, [2] a program that automates ML-related tasks such as data curation, hyperparameter optimization, and ML predictor generation. The combination of these programs allows for high-quality reaction energy profile studies and ML predictions to be generated with just a few command lines, starting from simple inputs such as databases with SMILES strings.

References

- [1] J. V. Alegre-Requena, S. Sowndarya, et al. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2023**, *13*, e1663.
- [2] J. V. Alegre-Requena, D. Dalmau. *ChemRxiv*, **2023**, DOI: 10.26434/chemrxiv-2023-k994h.