Reusable software for quantum chemistry applications

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The notion of reusable software libraries was around for a long time in the software development community. However, despite multiple advantages, a practice of reusing software is uncommon among computational chemists. We present *libefp* [1] – a full implementation of the effective fragment potential (EFP) method as a portable software library which brings reusable high-performance EFP implementation to the quantum chemistry community. The EFP method has emerged as a promising technique for performing simulations on extended molecular systems by substituting computationally expensive integral evaluations by first-principles derived formulas with parameters obtained from preparatory *ab initio* calculations. When electronic degrees of freedom are important, e.g., in case of a chemical reaction or electronic excitation, a part of the system where the electron rearrangement takes place can be described by quantum mechanical methods in a spirit of QM/MM schemes. *libefp* is the first software of its kind used by several major quantum chemistry packages such as NWChem [2], PSI4 [3], and Q-Chem [4] allowing a straightforward extension of unique electronic structure methodologies designed for accurate simulations in the gas phase to condensed phases via QM/EFP.

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2. Valiev, M. et al. Comput. Phys. Commun. 2010, 181, 1477-1489.
3. Turney, J.M. et al. Wiley Interdisciplinary Reviews: Computational Molecular Science 2012, 2, 556-565.
4. Shao, Y. et al. Phys. Chem. Chem. Phys. 2006, 8, 3172-3191.