Large-Scale Semiempirical Quantum Chemistry with EMPIRE

Johannes T. Margraf, Matthias Hennemann, Timothy Clark

Computer-Chemie-Centrum and Interdisciplinary Center for Molecular Materials, Department Chemie und Pharmazie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstrasse 25, 91052 Erlangen, Germany.

Atomistic simulations in biochemistry and materials science routinely involve large systems, consisting of thousands to millions of atoms. These simulations have mostly been restricted to methods using classical forcefields, which are usually unable to describe important electronic effects such as polarization, bond breaking or excitations. The semiempirical molecular orbital program EMPIRE allows the full quantum mechanical treatment of up to 100,000 atoms on massively-parallel computer architectures.[1] Thanks to EMPIRE's excellent scaling behavior on large clusters, even extremely large calculations can be performed without orbital-localization based linear-scaling algorithms. This is particularly important for the correct description of systems with small HOMO-LUMO gaps (i.e. semiconductors or zwitterionic proteins).[2]

In this talk, we will present some new functionalities of EMPIRE, which include periodic boundary conditions, molecular dynamics and dispersion corrections.[3] In combination, these extensions are highly promising for the study of complex condensed phase system such as liquids or amorphous molecular solids. We will also discuss some of the limitations of existing semiempirical methods and how they could be overcome.

[1] M. Hennemann and T. Clark, *J. Mol. Model.* **2014**, *20*, 2331.

[2] C. R. Wick, M. Hennemann, J. J. P. Stewart and T. Clark, *J. Mol. Model.* **2014**, *20*, 2159.

[3] J. T. Margraf, M. Hennemann, B. Meyer and T. Clark, *J. Mol. Model.* **2015**, *21*, 144.