GARLEEK: Adding an Extra Flavor to ONIOM

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ABSTRACT

The ONIOM method, developed in the group of Keiji Morokuma, is one of the most successful examples of quantum mechanics / molecular mechanics (QM/MM) treatments, and of multilayer methods in general. Its implementation in the Gaussian program package is in particular widely used. This implementation has access to the wide variety of QM methods available in Gaussian, but is limited to only three specific force fields. The current article presents the GARLEEK interface, which expands the availability of molecular mechanics methods to the wide variety of force fields available in the Tinker package. The focus is in the simple installation and use. Two examples of the performance of the interface with selected systems are provided. GARLEEK is MIT-licensed and freely available at https://github.com/insilichem/garleek.

Introduction

The application of distinct theoretical descriptions to different regions of the same system is a simple yet powerful concept in computational chemistry. This type of approach has been labeled as quantum mechanics/ molecular mechanics (QM/MM), multilayer or multiscale treatments. The popularity of the treatment was demonstrated by the Nobel Prize awarded to Karplus, Levitt and Warshel "for the development of multiscale models for complex chemical systems".[1–3] The original multilayer treatments in the 1960's and 1970's were of the QM/MM type, mostly in biological applications, and they were further developed through the 1980's.[4,5] An explosive expansion of the applications took place in the 1990's and has continued since, in part associated to increase in computational power, but also to methodological developments,[6–8] which have been summarized in more recent reviews.[9]

The contribution by Morokuma and co-workers was instrumental in the development of the field at that time, with the introduction of the "Integrated Molecular Orbital Molecular Mechanics" (IMOMM),[10] "Integrated Molecular Orbital Molecular Orbital" (IMOMO)[11] and, especially "Our own N-layered Integrated molecular Orbital and molecular Mechanics" (ONIOM)[12] methods. This work introduced the concept of substractive methods, where the low-level region is described not by a specific calculation, but by the substraction between low-level calculations on the full system and the high-level region. The use of a substractive scheme is a technical advantage, but does not modify the overall result.[12] The ONIOM method was implemented in the Gaussian98 version of the Gaussian package,[13] and has notably expanded the application of QM/MM methods beyond the range of biochemical systems.[14] A number of reviews can be found focused on applications in transition metal chemistry,[15]