The FGC approach for correcting noncovalent interactions in semiempirical quantum mechanical methods

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Noncovalent interactions play a fundamental role in many chemical and physical processes. For large molecular systems, practical calculations are limited to either semiempirical quantum mechanical (SQM) methods or molecular mechanical force fields. Traditionally, the most popular SQM methods are those based on the neglect of diatomic differential overlap (NDDO) approximation (e.g., the PM6 method). The dramatic approximations involved in these methods lead to substantial errors in the calculation of intermolecular interactions and, consequently, different approaches have been proposed to correct them [1]. More recently, the development of density functional tight binding (DFTB) has led to qualitative improvements in the accuracy of SQM methods [1,2]. Nevertheless, for many systems and depending on the orientations of the interacting molecules, the performance of SQM methods is still unsatisfactory, and therefore further efforts are required to improve them.

In this talk, we present a simple approach to improve the accuracy of SQM methods in the description of noncovalent interactions [4, 5]. Specifically, we use analytical, pairwise corrections in which the parameters depend on the nature of the interacting functional groups. An example of the successfulness of the method is displayed in Figure 1, where we compare interaction energies for 77 different complexes of the diglycine dimer, determined with the PM6 Hamiltonian, with our PM6-FGC method (FGC stands for functional group corrections) and, as a reference, with B3LYP-D3/def2-TZVP calculations. Our work shows the importance of including different orientations of the interacting molecules in the training set in order to obtain well-balanced pairwise corrections.

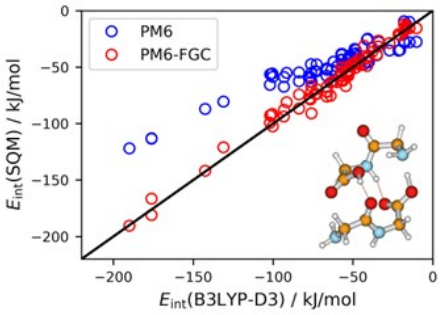

Figure 1: *Linear correlations between B3LYP-D3 interaction energies and those calculated with PM6 and PM6-FCG for conformers of the diglycine dimer.*

Index Terms: noncovalent interactions, semiempirical quantum mechanical methods.

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