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Comparison of ab initio MO, DFT and semi-empirical quantum chemical methods for computing biological molecules

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[INTRODUCTION] Recently, computer power has become large enough to compute any small or middle size molecules of interest, and most chemists can use quantum chemical computations for their studies. In various computational methods, density functional theory (DFT) method, particularly B3LYP method, is the most popular method because computational cost of DFT method is cheaper than of ab initio MO method although the latter is accurate in most molecular computations. On the other hand, for large molecules, semi-empirical quantum chemical method (semi-QM) could also be used, the computational cost of which is the cheapest in these methods. However, non-negligible disadvantages of DFT and semi-QM methods have also been reported to date. Moreover, various kinds of DFT methods, each of which has its own characteristics, are available. Here, we compare various DFT methods and semi-QM with ab initio MO method in several chemical properties for computing biological molecules.

[METHOD] First, we computed interaction energies between ammonia and formaldehyde with changing the distance between the molecules to evaluate hydrogen-bonding and van der Waals interaction by means of ab initio MO, such as MP2 and HF, DFT, such as B3LYP and M06-2X, and semi-QM methods, such as PM6-DH2. Secondly, we made Ramachandran diagrams using alanine model to evaluate the energy differences of amino acid with different main-chain dihedral angles by means of these methods. Next, we optimized the geometries of several polymers, such as poly-Ser, which are large biological molecules, and plotted those dihedral angles on the Ramachandran diagram. Finally, we computed dipole moments of poly-Gly and poly-Ala.

[RESULTS AND DISCUSSIONS] In the figure below, Ramachandran diagrams by MP2 method (left) and M06-2X method (right) are shown. The diagram by M06-2X is similar to the one by MP2 method. Moreover, we found that this trend is also valid for dipole moments. From these results, we conclude that M06-2X is the best method in the evaluated methods in the current work for calculating biological molecules.