Study of interaction energy analysis of proteins
by canonical Kohn-Sham molecular orbital calculation

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We have developed applications for canonical Kohn-Sham molecular orbitals (CMOs) calculation of proteins; *ProteinDF* [1] is a high-performance electronic structure calculation program, and *QCLObot* [2] is a provision, configuration management and creating precise initial guess tool for CMO calculations of protein.

As one of the properties obtained from the electronic states calculation results, the interaction energy analysis between amino acid residues and/or substrates is useful as protein design and functional analysis. Although the Morokuma method [3] is one of the well-known calculation methods for interaction energy analysis by using CMO calculations, the electronic structure calculation of large molecule is very expensive and hard to achieve in the first place. In this study, therefore, an interaction analysis program was developed based on the interaction analysis method using the energy density analysis (EDA) method [4].

To estimate the interaction energy based on this EDA method, the matrix element of the exchange-correlation term was necessary. So, the grid-free method [5, 6] was applied to evaluate the matrix elements of the exchange-correlation term in this study.

[1] https://github.com/ProteinDF/ProteinDF
[2] https://github.com/ProteinDF/QCLObot
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