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Shuang Ni
Wenbo Mo, Minjie Zhou
Laser Fusion Research Center, Chinese Academy of Engineering Physics, No. 64, Mianshan Road, Youxian District, Mianyang City, Sichuan Province, China
nishuang@163.com

Research on Intelligent Blocking Algorithm for Protein Raman Spectroscopy Based on Electron Density

Abstract

To address the key challenges in protein Raman spectral calculations, including the large number of atoms and the complexity of describing interactions in traditional blocking strategies, this study proposes a series of effective computational methods. First, based on the exciton model theoretical framework, a predictive model for protein Raman characteristic peaks was constructed. This model successfully predicted and classified the amide I and III characteristic peaks of four coronaviruses, with computational results matching experimental data, thereby fully validating the model's effectiveness[1].Considering the rapid advancements in supercomputing hardware and software, an innovative large-scale blocking strategy was proposed: by constructing "large fragment" blocking units of 200–400 atoms, the interactions of amino acid side chains were internalized within the blocks, forming a one-dimensional linear topological structure. This approach localized errors at the fragment ends and rigorously defined the concept of fragment error, proving that the total system error equals the fragment error[2,3].To further improve computational accuracy, an electron density-based adaptive segmentation algorithm was developed. This method achieves precise blocking by quantifying structural features and interaction strengths. Compared with traditional uniform segmentation approaches, the new algorithm significantly reduces the overall computational error by 20% while maintaining computational efficiency, through optimized handling of inter-fragment interactions[4].This study provides an efficient and reliable new approach for theoretical calculations of large-scale protein Raman spectra.

References

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Figures

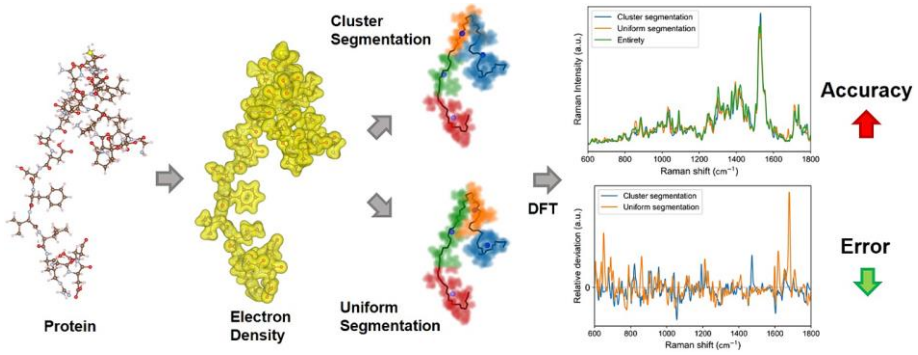

Figure 1: Schematic diagram of an intelligent block method based on electron density