Semiempirical molecular orbital calculations for 3d-4f complexes towards artificial metalloproteins

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Abstract

Because computational chemistry for proteins or metalloproteins, docking of ligands into proteins, and small molecules as ligands may require heavy calculations, low-precision but fast computational methods may be useful actually. Herein we introduce our preliminary results of semiempirical PM7 calculations for chiral Schiff base 3d-4f binuclear metal complexes containing many electrons.

Computational simulation of docking of ligands into proteins was used in drug design and discovery in silico commonly. Moreover, metal complexes as well as organic ligands were also treated in new study on protein surface mimetics¹ besides purely biochemical protein-protein interactions.² Recently, not only docking programs such as GOLD³, the PM6 semi-empirical method was applied to modeling proteins for enhancing docking accuracy⁴. Of course, proteins are large systems composed of many atoms. However, even ligands may be many electron systems when a ligand contains heavy metal atoms such as third transition metals or lanthanide metals. Indeed, we have reported on fluorescence, UV-vis and CD spectral changes by docking of chiral Schiff base 3d (zinc(II)) or the related 3d-4f complexes into lysozyme or HSA proteins experimentally⁵. Furthermore, in the course work of organic/inorganic hybrid materials, we have begun to prepare artificial metalloproteins by using various proteins and metal complexes. Here we show results of calculation of the analogous 3d-4f complexes^{6,7} not by precise TD-DFT methods but by semiempirical molecular orbital method Sparkle/PM7⁸ and ORCA⁹ in a MOPAC2012 package mainly to obtain optimized structures (Fig. 1) towards protein-ligand interaction and simulated UV-vis spectra theoretically (Fig. 2). As for Nd(III)-Cu(II) complex, differences of coordination bond distances between crystal structures and calculations were less than 0.0746 and 0.0286 nm for Cu(II) and Nd(III) coordination environments, respectively. The corresponding values are 0.0027 and 0.0594 nm for La(III)-Ni(II) complex, 0.00050 and 0.0489 nm for La(III)-Cu(II) complex, and 0.0053 and 0.0486 nm for Nd(III)-Ni(II) complex, respectively. Thus acceptable results in structures could be also obtained in considerably shorter time than TD-DFT regardless of so many 4f-electron systems.

Fig. 1. Optimized structure of Nd(III)-Cu(II) complex.

Fig. 2. Experimental (green broken line) and simulated (blue solid line) UV-vis spectra of Nd(III)-Cu(II) complex.

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