Electronic structure of the active site on glucose oxidase by using canonical molecular orbital calculation

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Glucose oxidase (GOx) is an enzyme which catalyzes the oxidation of beta-D-glucose to D-glucono-1,5-lactone, and has been widely used in some glucose meters. In order to characterize the electronic structure around the active site and interactions among residues, we have carried out the canonical molecular (CMO) calculations of the GOx models based on DFT. In this report, we show the computational procedure of the CMO for the GOx protein, and the electronic structure around the active site, the flavin adenine dinucleotide (FAD; oxidation state) and FADH2 (reduced state).

The computation model of the GOx was formed on the basis of the experimental structure data (PDB accession code 3QVP [1]). The CMO computational models were gained by extracting the FAD and surrounding amino acid residues within 2, 3, 4 and 5 Å from the FAD. The CMO calculations were performed by using our program, ProteinDF and QCLObot [2]. The computation results of the electronic structures (Fig.1) indicated that the surrounding amino acids (AA) brought about the environments in which the FAD was easily reduced to the FADH2.

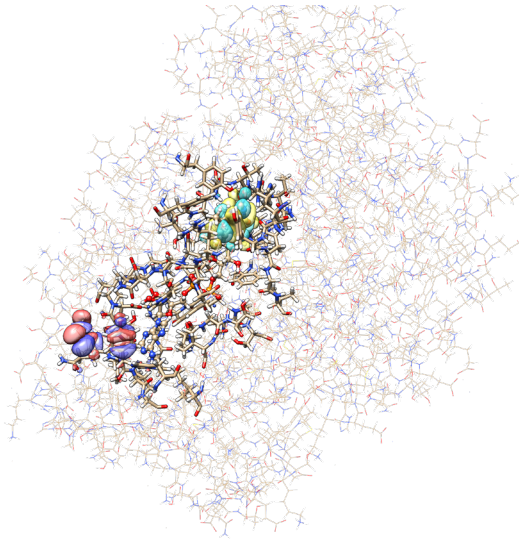

Fig. 1. The HOMO (red, blue) and LUMO (yellow, green) of the model (FAD + 5Å A.A.)

[1] Kommoju, P.R., Chen, Z.W., Bruckner, R.C., Mathews, F.S., Jorns, M.S., *Biochemistry*, **50**, 5521-5534, (2011).
[2] http://proteindf.github.io/