Takashiro Akitsu et al., Biochem Anal Biochem 2016, 5:5(Suppl)
http://dx.doi.org/10.4172/2161-1009.C1.012

Computational study of Cu(II) complexes with the condensation product of salicylaldehyde and L-aspartic acid

Takashiro Akitsu[1], Arshak Tsaturyan[2], Igor Shcherbakov[2] and Nanami Yoshida[1]
[1]Tokyo University of Science, Japan
[2]Southern Federal University, Russia

Copper(II) and zinc(II) complexes with Schiff bases of *L*-amino acids and their hybrid materials containing titanium(IV) oxide have potential applications for DSSC dyes, photocatalysis, or sunscreen cosmetics. Since, the structures and reactions in solutions of these systems are not fully explored, we carried out computational study on copper(II/I) complexes to give insight in the stability of estimated forms, thermodynamical parameters, redox potentials, absorption spectra and molecular orbitals. For example, reactions of formation of four-methanolysis Cu(II/I) complexes were examined by the means of DFT method. The stability of complexes with three and tetradentate coordination surrondings of metal centers was estimated on the basis of ΔG of formations. According to the results, Cu(II) complex has square-planar geometry. Redox potential was calculated from Born-Haber cycle. The absorption spectra of Cu(II) complexes were modeled by TD-DFT calculation in methanol solution using optimized geometry. The electronic transitions for [$CuLCH_3OH$] are red shifted compared with [CuL].

Biography

Takashiro Akitsu has completed his PhD from Department of Chemistry, Osaka University and Post-doctoral studies from Institute for Protein Research, Osaka University. He is currently working as a Professor of Department of Chemistry, Faculty of Science, Tokyo University of Science. He has published more than 140 papers in reputed journals and has been serving as an Editorial Board Member.

akitsu@rs.kagu.tus.ac.jp