F. Sato LAB.

[Innovative Simulation on Proteins]

Center for Research on Innovative Simulation Software

http://www.ciss.iis.u-tokyo.ac.jp, http://satolab.iis.u-tokyo.ac.jp

Computational Biomolecular Science

Engineering/
Mechanical Engineering

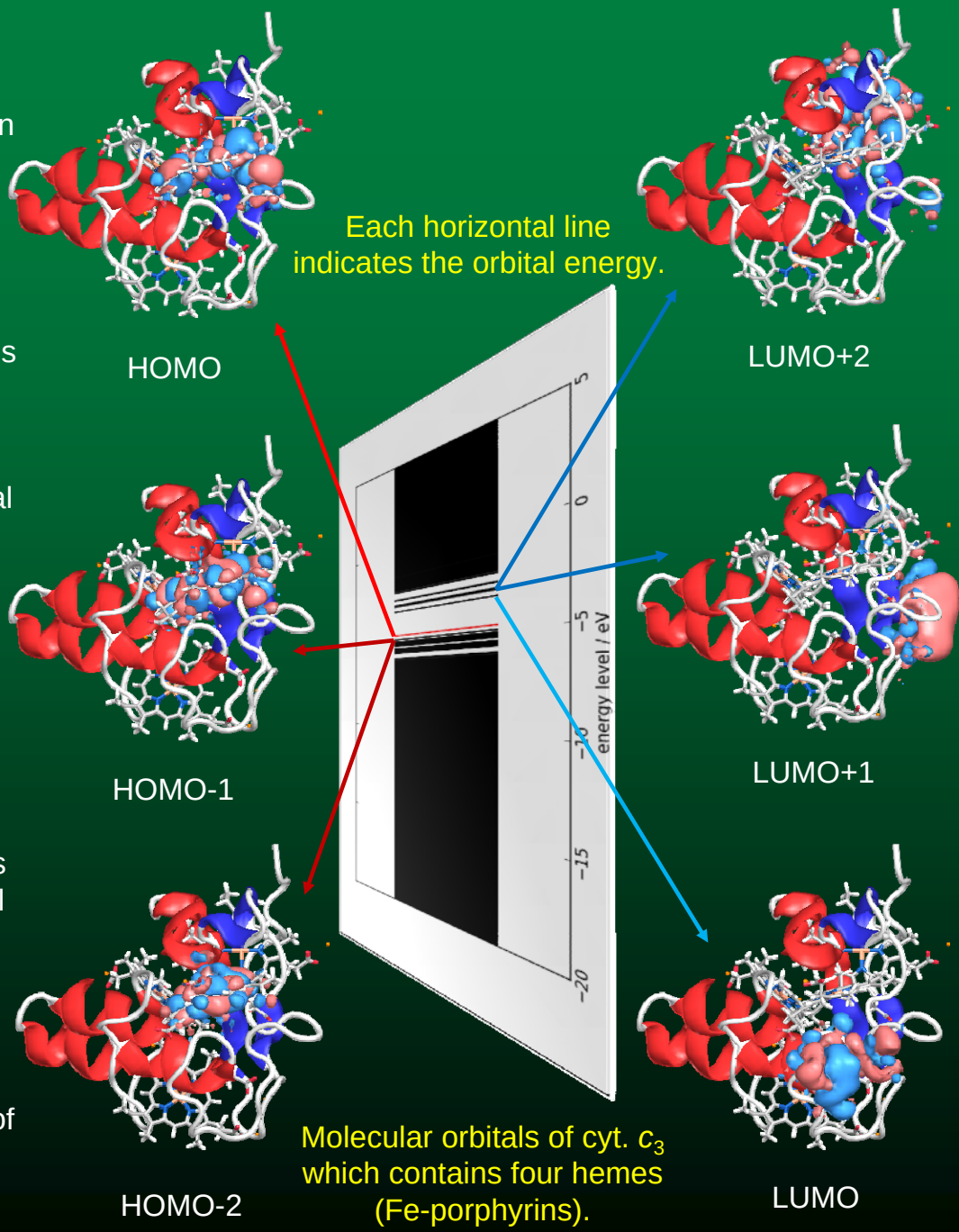
All-Electron Calculations on Proteins by ProteinDF

All-Electron Calculations on Proteins by ProteinDF

The new quantum chemical calculation software "ProteinDF" was developed, where molecular orbitals of all electrons of proteins are computable.

Based on the software, a practical simulation system that precisely analyzes biomolecular reactions is now constructed for the applied research such as design of new enzyme and medicine as well as for the fundamental research.

Please enjoy the world of beautiful molecular orbitals of protein.



Molecular orbitals of cyt. c_3 which contains four hemes (Fe-porphyrins).