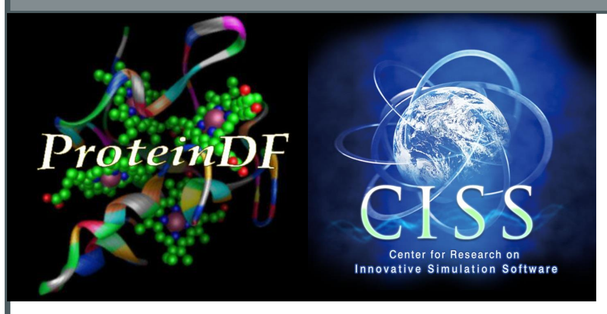


F. SATO LAB.

[Innovative Simulation of Bio and Nano Molecules]

Center for Research on Innovative Simulation Software

Computational Biomolecular Science

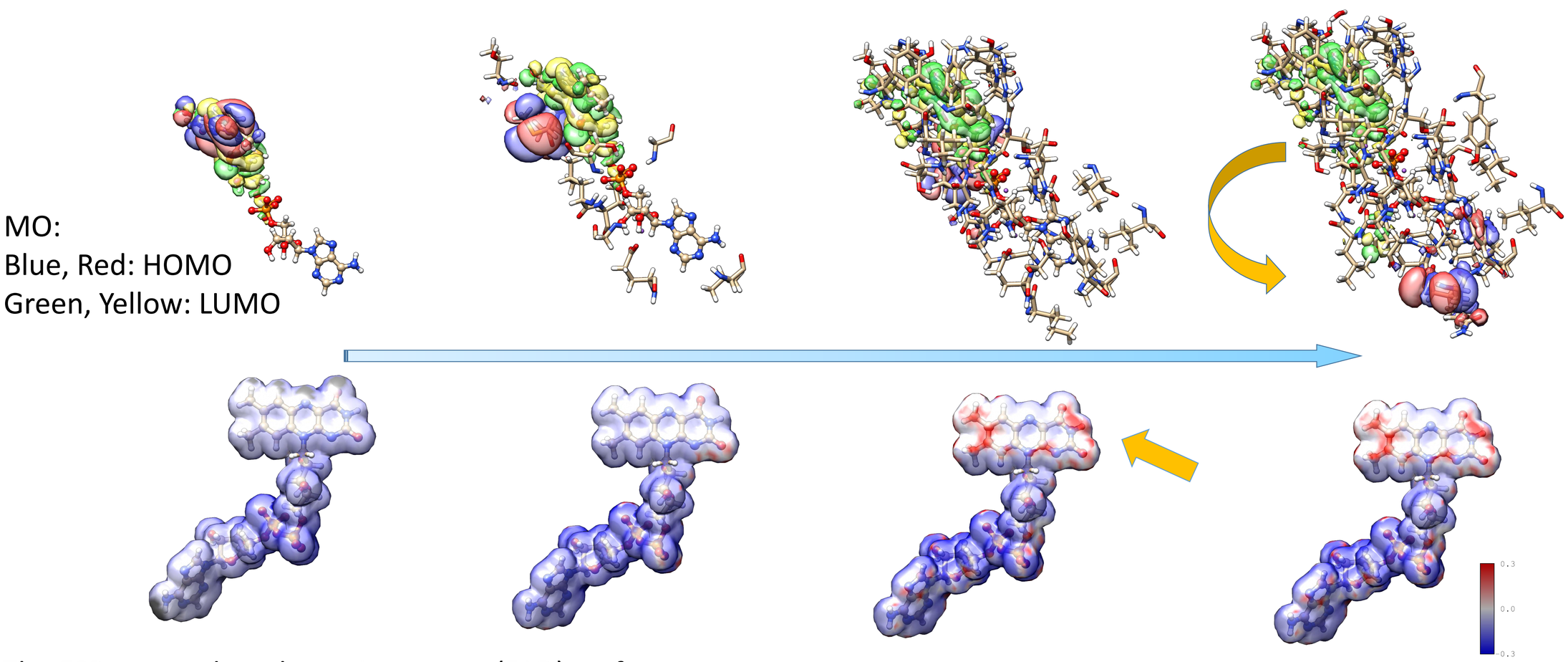
Mechanical Engineering department

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

Large-Scale Canonical Molecular Orbitals Study

Has Great Potential in Shaping the Future.

The new quantum chemical calculation software “ProteinDF” has been developed, where canonical molecular orbitals of all electrons of nanoscale molecules such as proteins are computable. https://github.com/ProteinDF/



The ESP mapped on the active center (FAD) surface

Typical Roles of Electrons in Protein

Textbooks (Japanese)