# F. SATO LAB.

## [ Innovative Simulation of Bio and Nano Molecules ]

**Center for Research on Innovative Simulation Software**

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

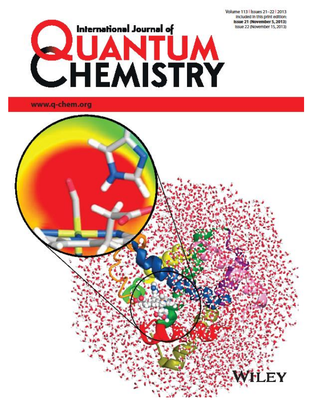
**Engineering/ Mechanical Engineering**

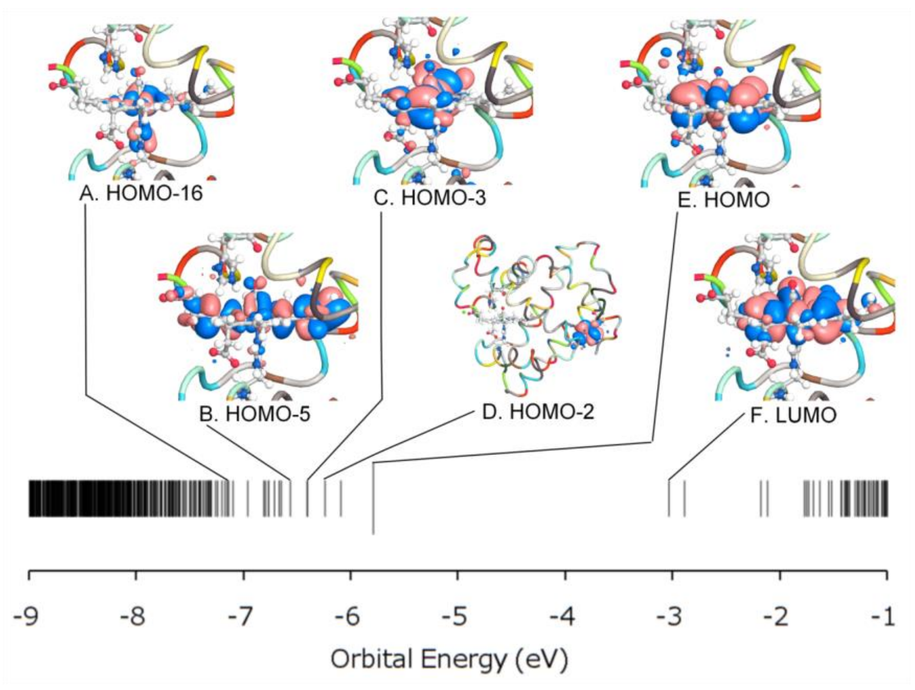
**Computational Biomolecular Science**

## Large-Scale Canonical Molecular Orbitals Study

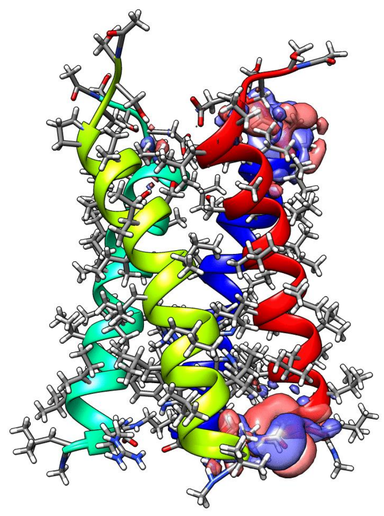
**Has Great Potential in Shaping the Future.**

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.




All-electron calculation
of metal-containing protein



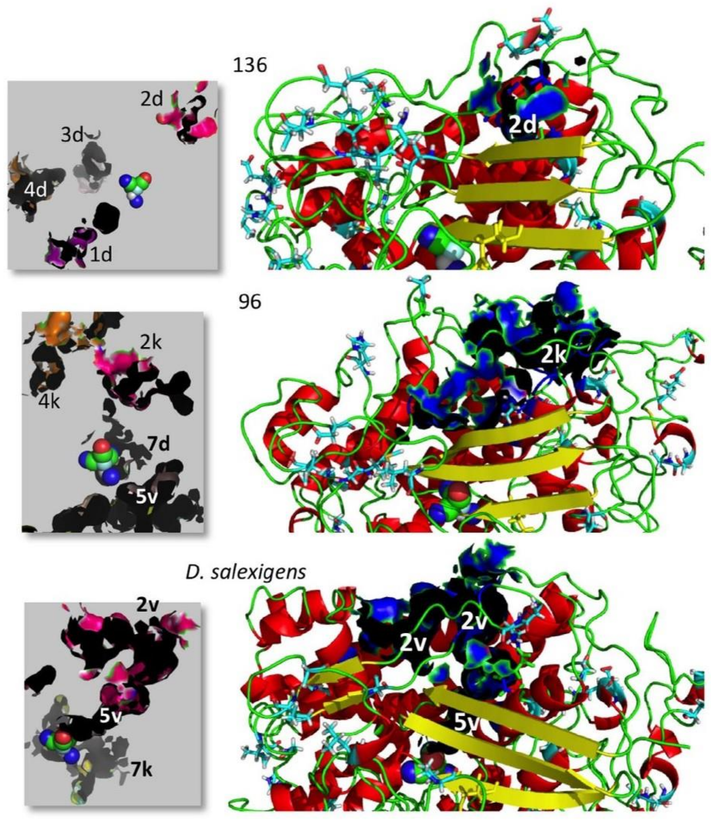
First-principle MD
of proton-channel protein


- T. Hirano, F. Sato, *PCCP,* 2014, **16**, 14496.
- K. Chiba, T. Hirano, F. Sato, M. Okamoto, *IJQC,* 2013, **113**, 2345.

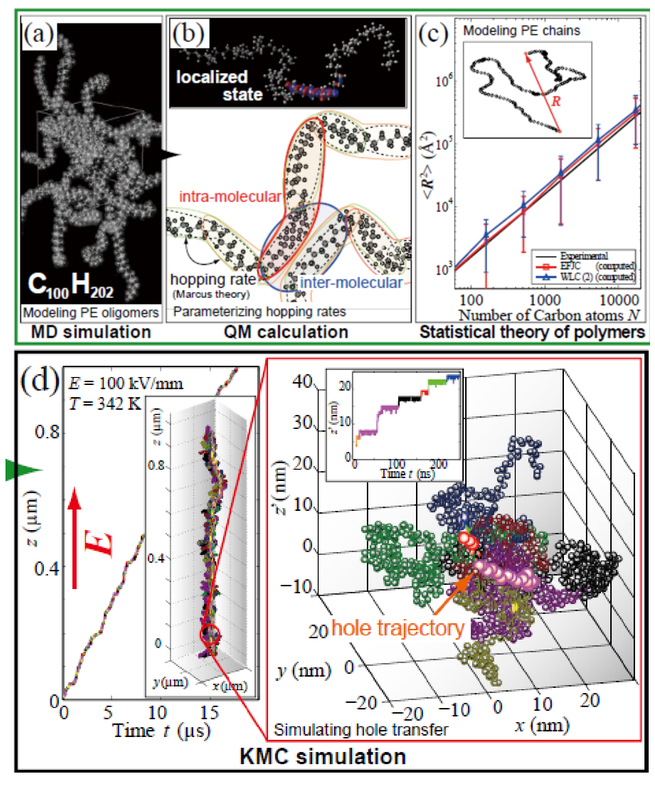


Textbooks (Japanese)

### Various applied researches




Prediction of gas-cavity structure
in [Ni-Fe-Se] hydrogenase




Analysis of electron mobility
in insulating material


- T. Tamura, N. Tsunekawa, M. Nemoto, K. Inagaki, T. Hirano, F. Sato, *Sci. Rep*., 2016, **6**, 19742.
- M. Sato, A. Kumada, K. Hidaka, T. Hirano, F. Sato, *JPC. C,* 2016, jp6b01581.