F. SATO LAB.

Innovative Simulation of Bio and Nano Molecules

Center for Research on Innovative Simulation Software

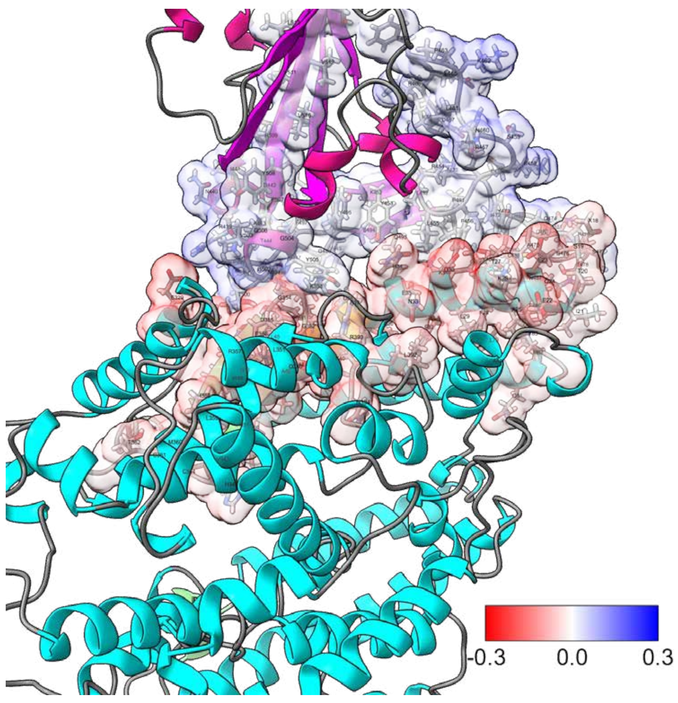
Computational Biomolecular Science

Department of Mechanical Engineering, Graduate School of Engineering

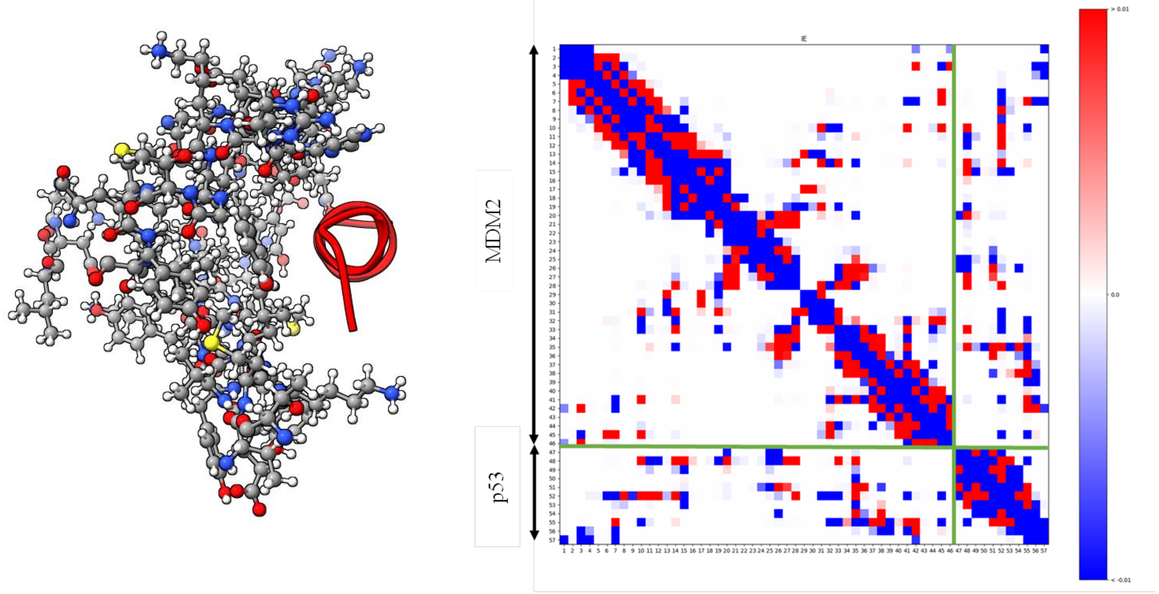
http://www.satolab.iis.u-tokyo.ac.jp/
http://www.ciss.iis.u-tokyo.ac.jp/

Protein Design Using Quantum Chemical Calculation

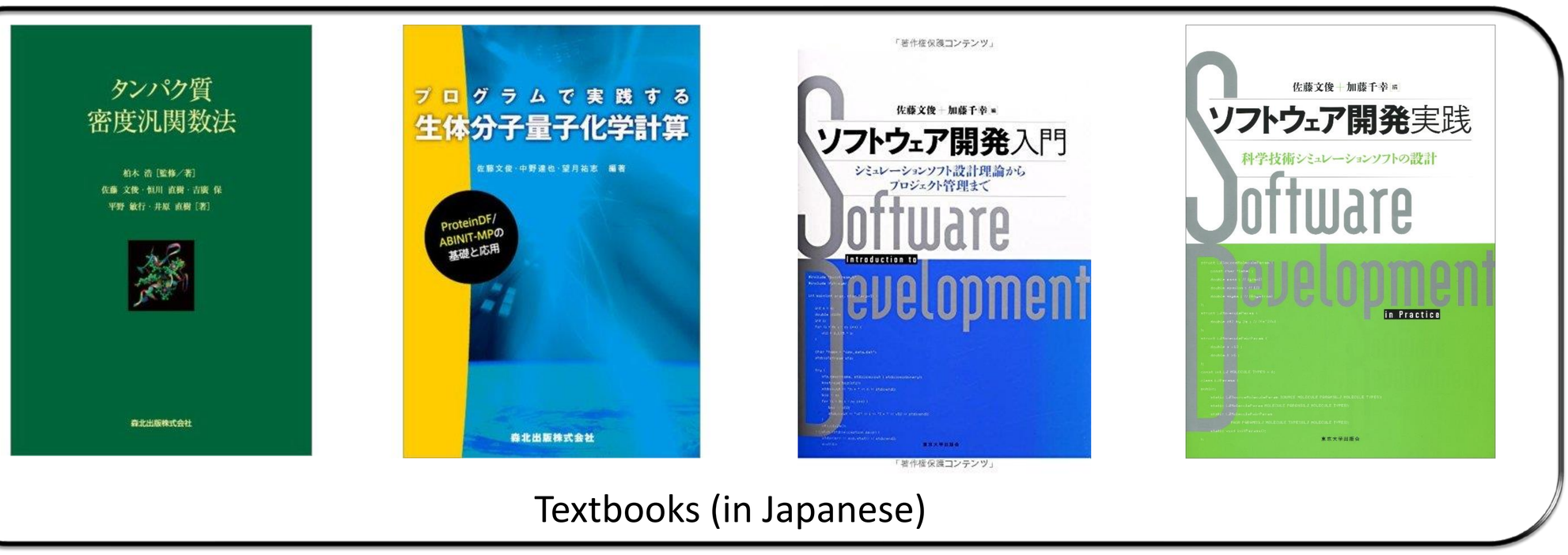
Our group has been developing the quantum chemical calculation software "ProteinDF/QCLObot" which can calculate all canonical molecular orbitals of proteins.
https://proteindf.github.io/
We are using these software to analyze and design the electronic structure proteins.



Electrostatic potential distribution of SARS-CoV-2 viral spike protein (upper side) and ACE2 (its lower side) in the binding region



(left) Structure of p53-MDM2 complex model. p53-derived peptide is shown in red.
(right) Heatmap of interaction energy in the complex model



Textbooks (in Japanese)