THE UNIVERSITY OF TOKYO

ISLiM Integrated Simulation of Living Matter | RISS Research and Development of Innovative Simulation Software | CISS Center for Research on Innovative Simulation Software

All-Electron Wave-function Calculations of Proteins by DFT

ProteinDF

ProteinDF System

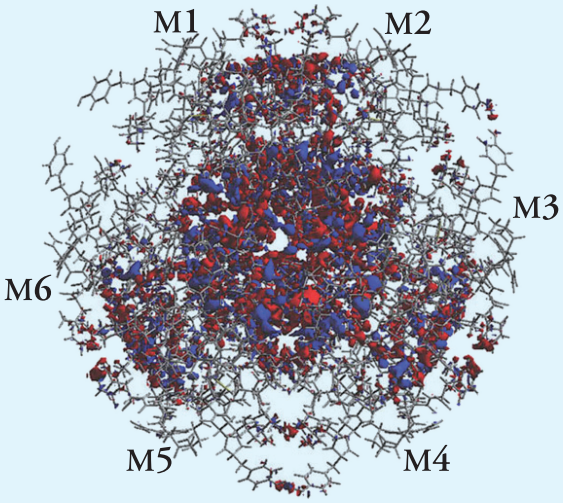
Up-to-date functions for electronic modeling of biomolecules

From PC clusters to supercomputers

Standard DFT program using Gaussian basis sets

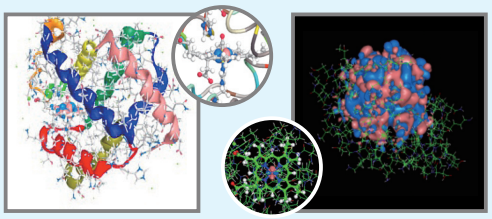
Feasibility Studies

Large calculations

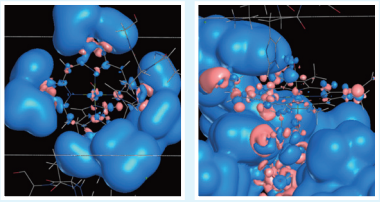


Difference electron density map
for insulin hexamer and 6 monomers
✔ Electron redistribution to stabilize hexamer

(Metallo-) Protein calculations

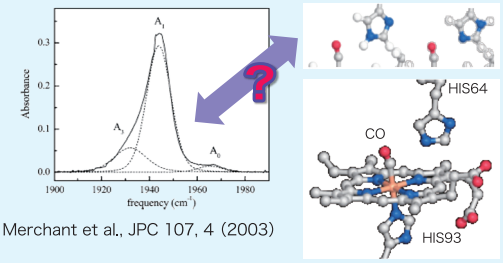


Molecular orbitals of hemeproteins. (left) MbCO, (right) Cyt. *c*
✔ The functions of the proteins are reflected



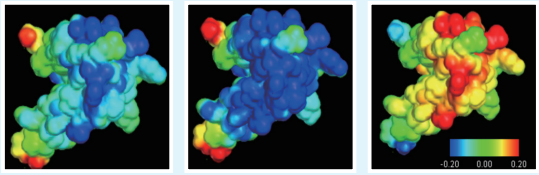
Difference electron density map
(left) substitution of side-chain (porphyrin → protoporphyrin)
(right) increase of peptide size (3 → 14 residues)
✔ Roles of electrons in proteins

Molecular properties



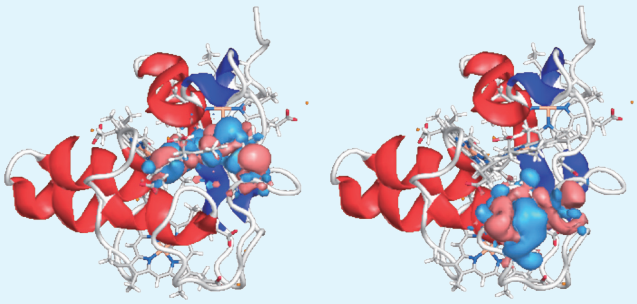
Merchant et al., JPC 107, 4 (2003)

IR spectrum identification of CO stretching frequency in MbCO
✔ Analysis and forecast of experiment values

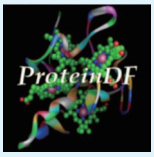


The electrostatic potential (ESP) map of insulin
(left) all-electron, (middle) conventional calculations,
and (right) difference map between them
✔ Precise ESP calculations

Complex proteins



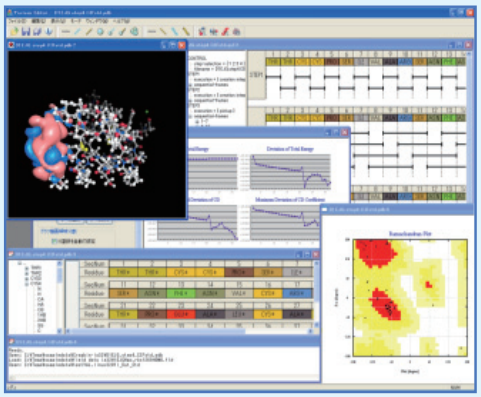
Molecular orbital of Cyt. c_3
(left) HOMO, (right) LUMO
✔ The complex protein that contains four hemes



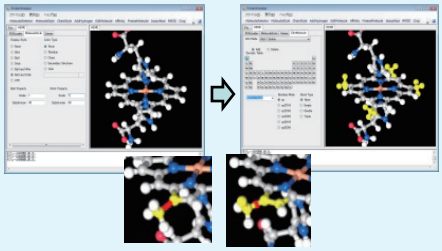
Tips:
Cyt. c_3 is used as
the logo of ProteinDF.

References (Japanese)
ISBN-13: 978-4627241411, ISBN-13: 978-4627879119

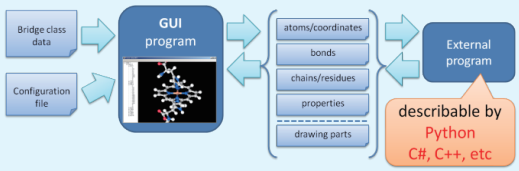
Pre/Post Environment



Snapshot of ProteinEditor



Molecular modeling (under construction)



Concept of customization of pre/post environment

In all-electron calculations on proteins, the volume of data is huge and the simulation is very complex.

ProteinEditor is a pre/post tool to assist with the protein quantum chemical calculation.

From the 2011 version, the data structure has been changed to an independent platform. It is possible to use it as an interactive environment and/or its own external program by describing the codes.

Functions

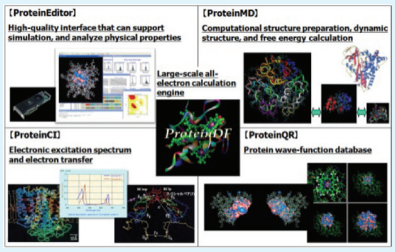
Functions	Contents (including those under construction)
All-electron canonical molecular orbital calculation	Direct SCF, Resolution of Identity (RI) method
Computational methods	SVWN/BLYP/B3LYP/DFT+D/LC/CAM-B3LYP, HF, Dual-level DFT
Convergence techniques	Simple/Anderson/DIIS/Projection/ Level-shift/MO overlap methods
Molecular properties	Molecular orbital, Electron density, Electrostatic potential, EDA, IR/Raman Energy (ground/excited/gradient) Geometry optimization, NMR
Basis sets	DZV/DZVP/DZVP2, Optimized Fe basis set, etc.

Modules	Advanced characters (including those under construction)
ProteinDF	Massively parallel control over 10,000 cores Molecular properties calculations
QCLO	Semi-automatic solver for the all-electron canonical molecular orbital calculation of peptides
ProteinMD	DFT-MD/DFT-MC Geometry optimization (and IRC)
ProteinCI	Grimme DFT-CI, HF-CIS
ProteinEditor	Pre/post environment for the all-electron calculations on biomolecules Molecular modeling, Interactive GUI Customizable as the external program
ProteinQR	Protein wave-function database

Platforms

OS: UNIX/Linux (Redhat, SuSE, Ubuntu), C++ compiler: gcc/intel/PGI
Libraries: MPI, LAPACK/ScaLAPACK
Computers: SGI Altix, Cray XT, Fujitsu PRIMERGY, HA8000 (T2K)
Front-end (ProteinEditor): Windows XP/Vista/7

ProteinDF package



The ProteinDF system consists of ProteinDF /QCLO, ProteinMD, ProteinCI, ProteinQR, and ProteinEditor modules.

A simulation that cooperates between each module can be executed.

Documents

Install/Users manuals
Tutorial guide, samples

Future works

New functions : CD method, NMR chemical shift, large geometry optimization
Improvement : energy gradient, DFT-MD, DFT-CI, EDA
Under porting for the next generation "K" supercomputer.

ProteinDF is supported by the "Research and Development of Innovative Simulation Software (RISS)" and "Next-Generation Integrated Simulation of Living Matter (ISLiM)" projects.

Please contact us if you would like to use or customize this software.
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http://satolab.iis.u-tokyo.ac.jp/

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