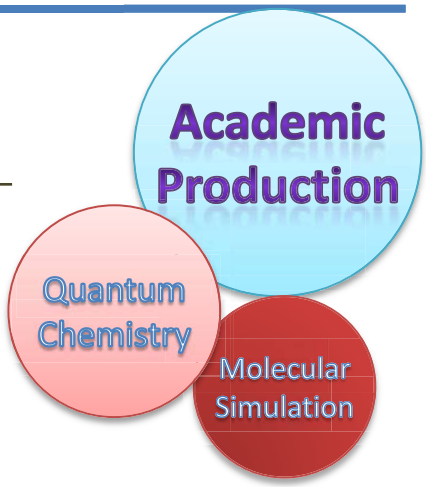
MORI, Hirotoshi

Division of Advanced Sciences, Ocha-dai Academic Production

http://web.me.com/qc_forest/SimulationScienceLab/Home.html



■ **Researcher information**

Contact

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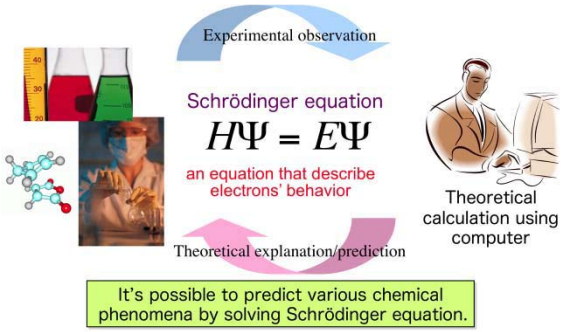
Major

Theoretical & Computational Chemistry, Quantum Chemistry

■ **Research topics**

Development of large-scale molecular theories and their applications to engineering/biochemistry



Keywords

Molecular Simulation, Relativistic Molecular Orbital Calculation, Molecular Dynamics, Functional & Bio-molecules, Metals

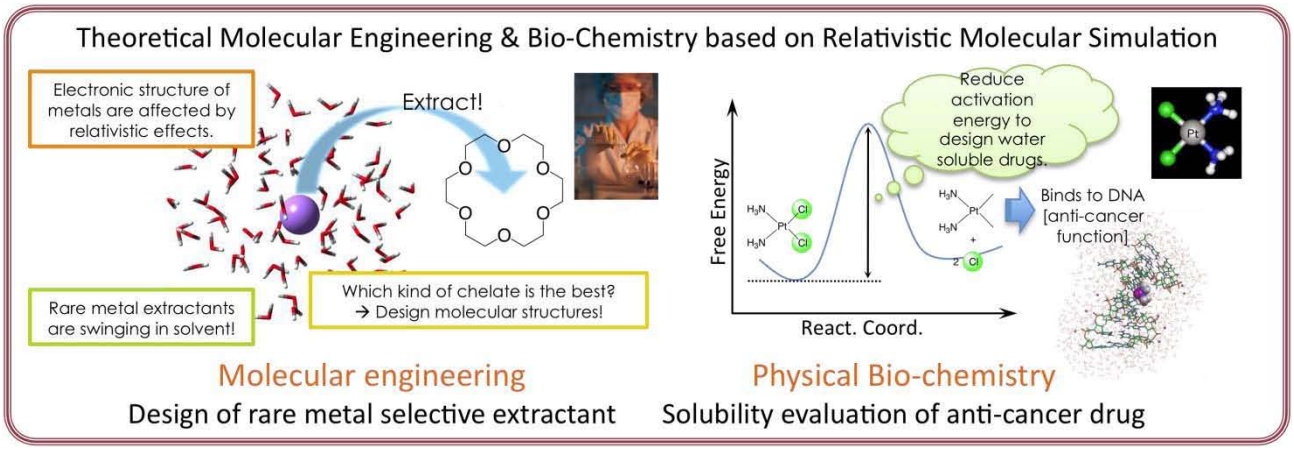
Contents

■ Overview (background, goal, detail)

Developing relativistic quantum chemical methods and using molecular dynamics technique, we're designing functional materials and studying functions of bio-molecules containing metal elements. We're tackling the complicated (but interesting & important) metal-chemistry from theoretical point of view.

■ Process, case study

1) Developments of relativistic quantum molecular theories for molecular simulations containing heavy metal elements
2) Theoretical design of rare metal selective extractant
3) Ab initio molecular dynamics simulations of anti-cancer drugs: theoretical evaluation of water solubility



Intellectual properties (Patents, computer programs), productization, publications and social/industrial contributions

・Contributions to Quantum Chemical Program Packages (Developments of relativistic model core potential method for heavy elements)
ABINIT-MPX
GAMESS

Potential of social/industrial contribution

■ Joint research/ licensing / technical consulting / knowledge sharing (open courses, workshops, publications)

Joint research relating with theoretical molecular design based on quantum molecular theory will be possible.