Elongation method for efficient quantum chemistry calculations toward functional designs of bio/nano materials

Yuriko Aoki, Wataru Mizukami, Ikuko Okawa, Yuuichi Orimoto
(Faculty of Engineering Sciences, Kyushu University)

Toward exact ab initio computations by Order(N)

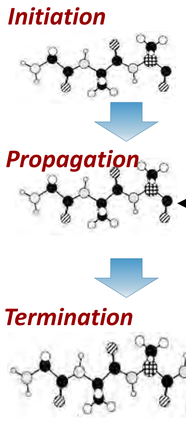
Elongation method

To calculate electronic states of a gigantic system, the computational time increases with Order N^4 (N : number of atoms). The elongation method developed by our group enables efficient calculations by connecting units successively in a similar way as polymeric polymerization reaction, and calculates only reaction sites considering whole electronic states.

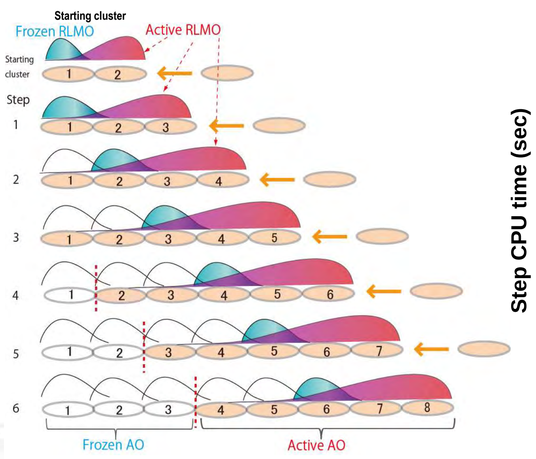
Theoretical synthesis of polymers

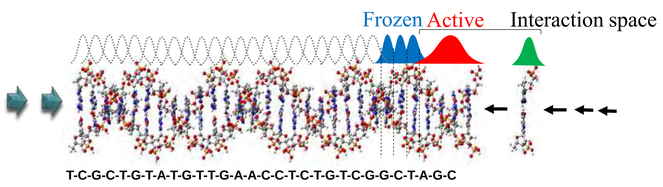
Elongation (ELG) method

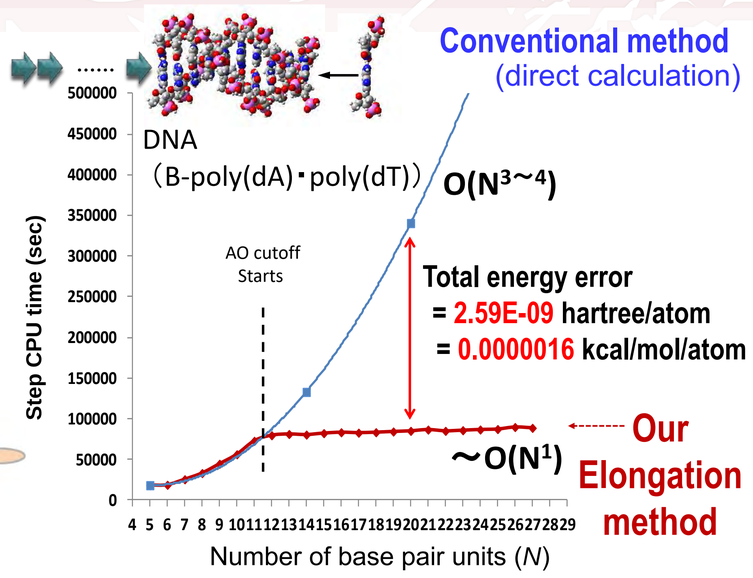
Computational polymerization



Region localized molecular orbitals (RLMOs)







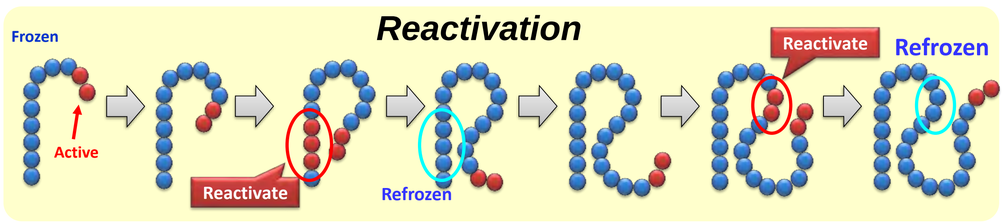
- **Order (N) efficient calculations**
- **Chemical accuracy retained for huge systems**

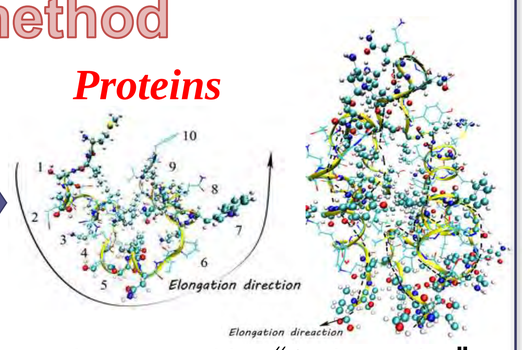
The calculation speed is proportional to the linear scaling of the system size (Order N method). Nonetheless, the calculation precision is very accurate with an energy error of 10^{-8} Hartree/atom or less compared to the conventional method, and even when considering a gigantic system consisting of 10^5 atoms (for example, chaperone protein…about 120,000 atoms) , those errors can be only within chemical accuracy.

Besides, since only the reactive sites are calculated, necessary memory and disk capacity are small, so the system with large size, which could not be treated by conventional method, can be calculated efficiently by elongation method.

3D (Three dimensional) - Elongation method

・・・one by one activation





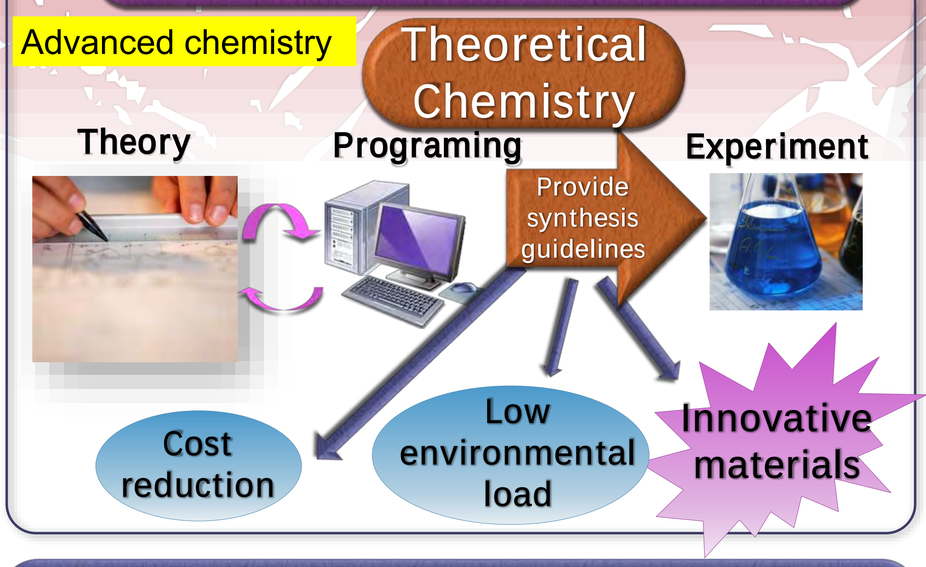
Any dimension systems can be calculated by thawing the "Frozen region" according to the approaching "Active region" while retaining the concept of one dimensional expansion which calculates only the reactive part.

Ancient chemistry

Explore materials only by experimental alchemists

Design & prediction of new materials

Advanced chemistry



Rare-metal free magnetic polymer design

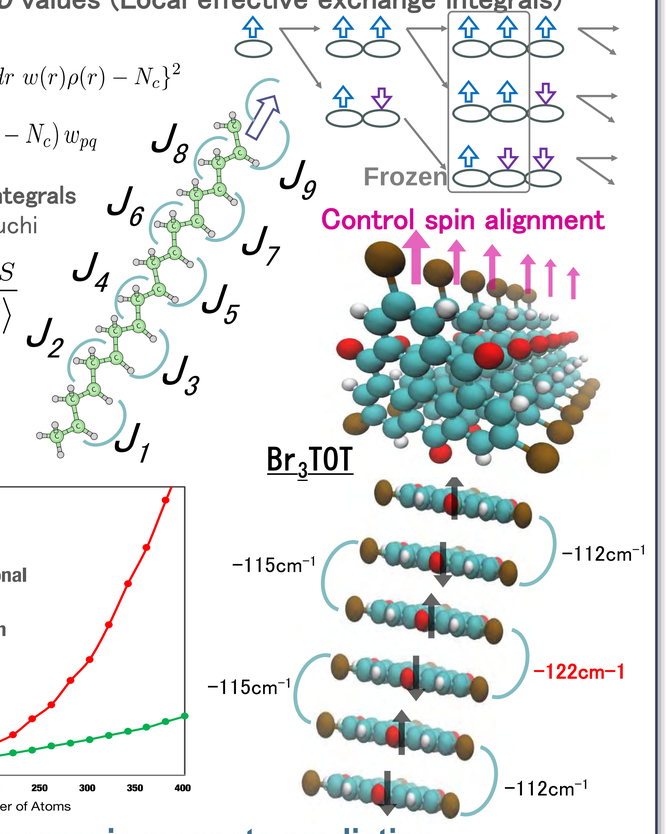
By restrained DFT + Elongation method
Prediction of J values (Local effective exchange integrals)

$$\tilde{E}[\rho] = E[\rho] + \frac{1}{2}V\{\int dr\ w(r)\rho(r) - N_c\}^2$$

$$\tilde{F}_{pq} = F_{pq} + V\,\mathrm{Tr}\,(\mathbf{wD} - N_c)\,w_{pq}$$

Effective exchange integrals
by Yamaguchi

$$J = \frac{E_{LS} - E_{HS}}{4\langle S_A\rangle\langle S_B\rangle}$$

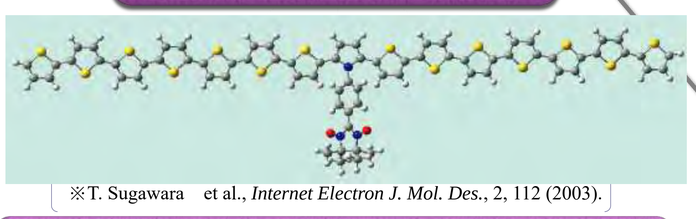


Useful for organic magnets prediction

New material design using quantum chemistry & supercomputer

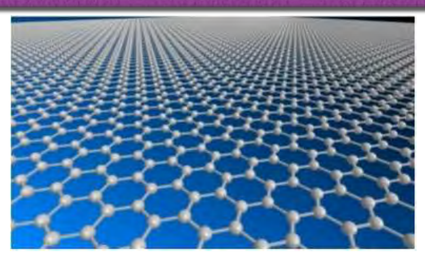
We developed the unique theory and method – Elongation method – applicable gigantic bio/nano systems which were impossible to be treated by conventional method. The computational accuracy of elongation method provides high precision, and the computational efficiency is linear scaling. By means of the material designs from a microscopic viewpoint, we aim to contribute our novel approach to green & life innovation, rare metal substitution problems, nanotechnology using IT, and so on.

(quasi) 1 D system …Molecular Wire

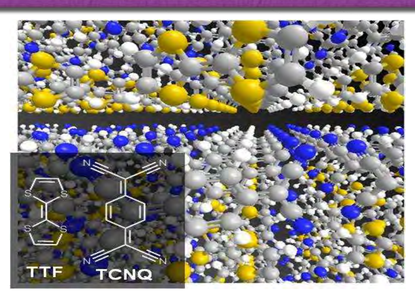


※T. Sugawara et al., *Internet Electron J. Mol. Des.*, 2, 112 (2003).

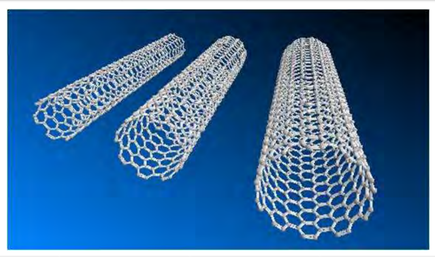
2 D system…Molecular Sheet



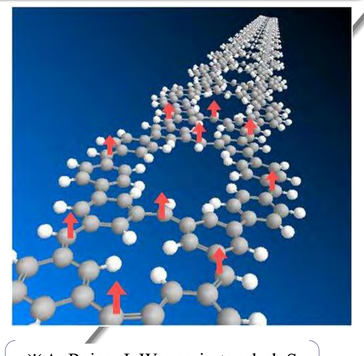
3 D system…crystal



Conductivity of nanotubes (conductor/semiconductor)

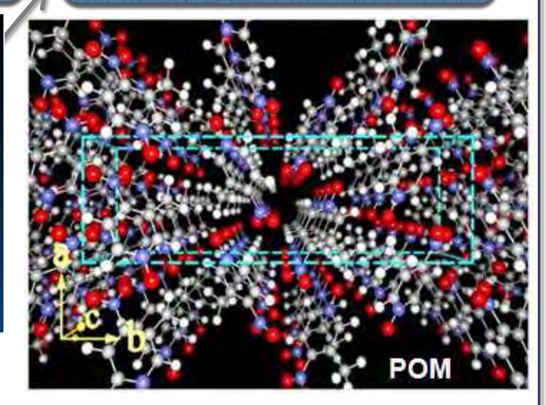


Organic ferromagnetic polymers



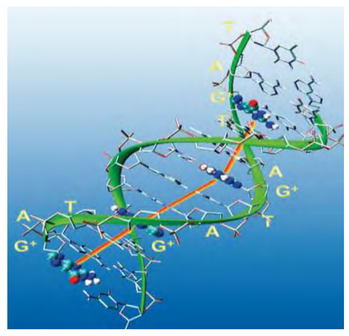
※A. Rajca, J. Wongsriratanakul, S. Rajca, *Science*, **294**, 1503 (2001).

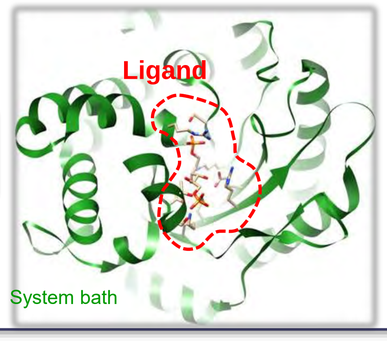
Non-linear optical property



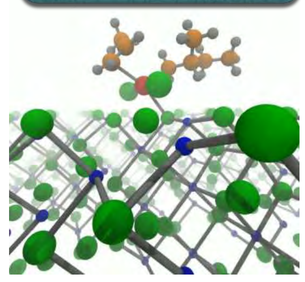
Our original theory & method & applications
- Elongation Method
- Through space/bond analysis
- Organic ferromagnetic analysis
- Non-liner optical property analysis
- Conductivity analysis
- Catalytic reaction analysis

Biological molecules





Catalytic reactions



Organic solar battery