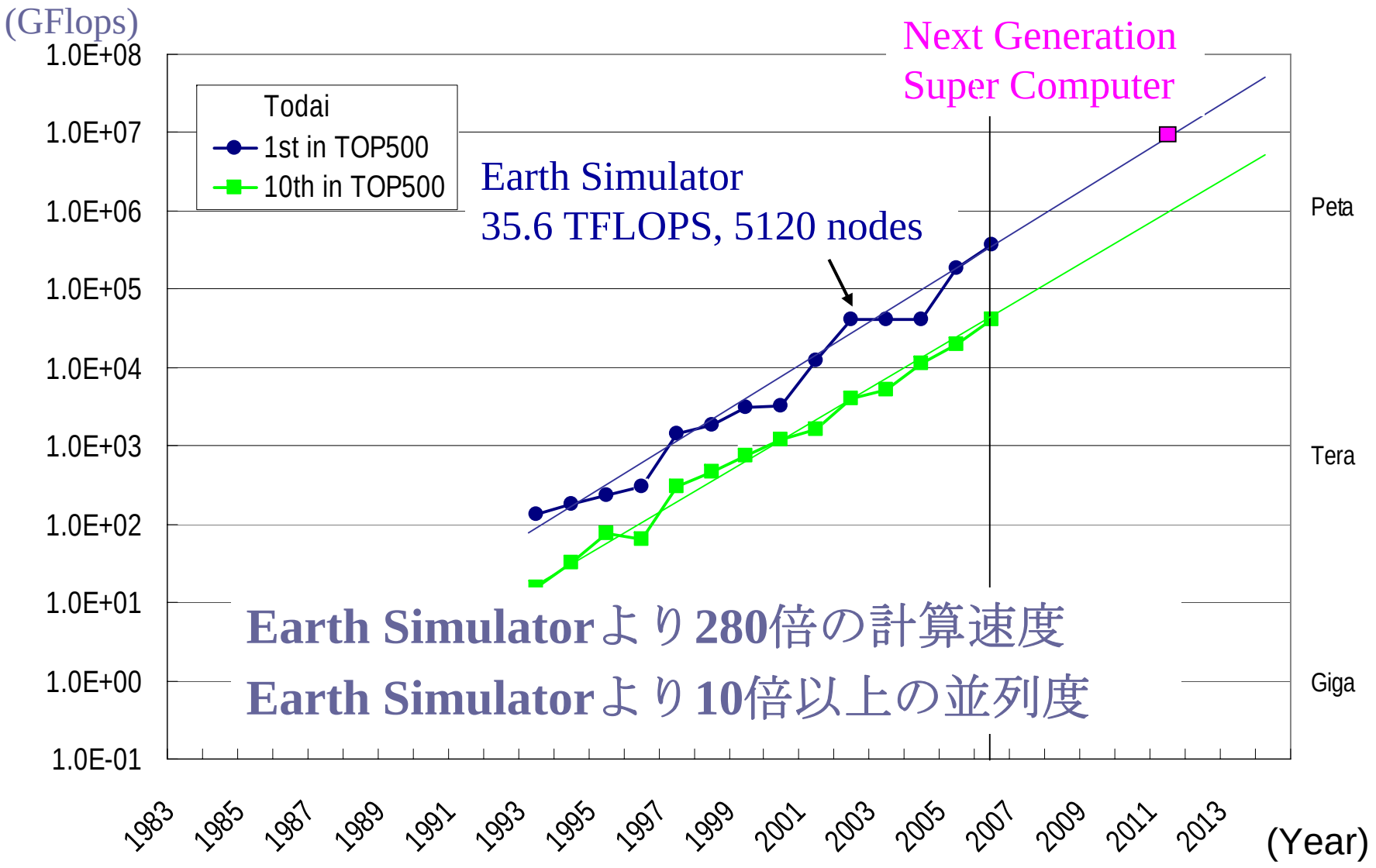
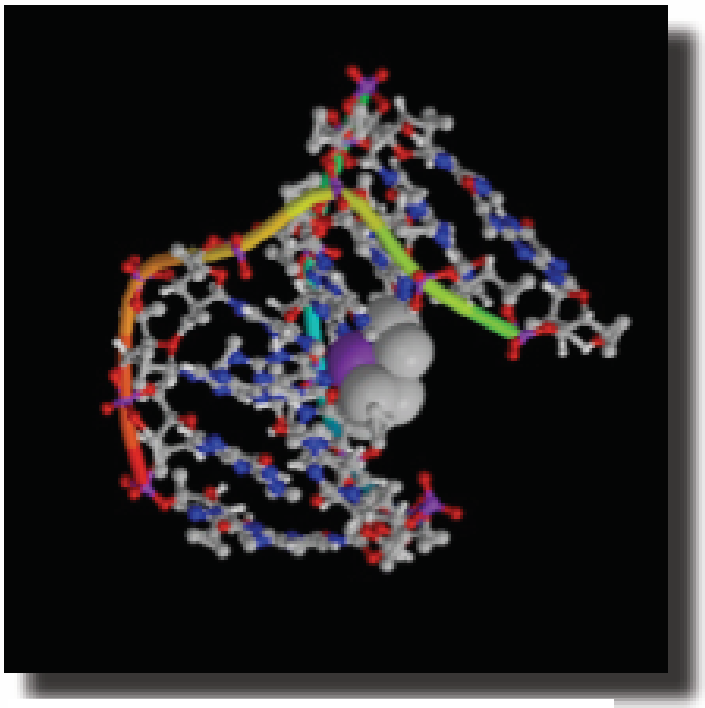
Next Generation Supercomputer Project

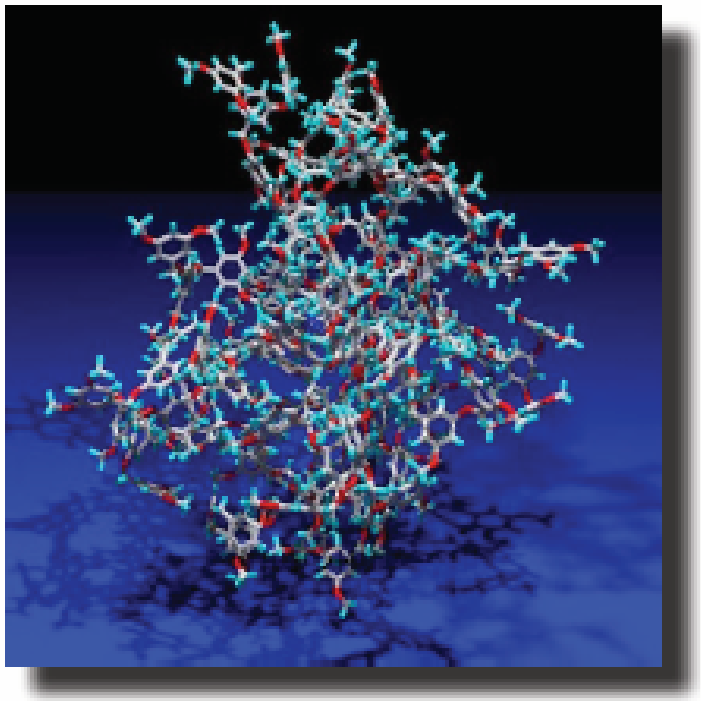


Nano-Bio Simulation

With the emergence of petascale computing platforms computational chemistry is on the verge of entering a new era of modeling. It will enable us to tackle scientific problems that larger and more complex, more realistic than ever before, and to include more of the complex dynamical behavior of nature. Petascale computing should be science driven.



Biomolecules



Nano-scale molecules

- Simulations for larger and more complex, more realistic systems
- Very Accurate results
- Chemistry at periodic interfaces
- Coupling multiple scales
- Benchmarking abilities
- Heavy element chemistry

大規模分子系への理論化学の展開

- 波動関数法（*ab initio* MO法）

  体系的理論、近似を上げれば厳密解に収束
  小さな系では極めて精度の高い結果を与える
  計算時間の系の大きさ(*N*)依存性が大きい（計算時間がかかりすぎる）

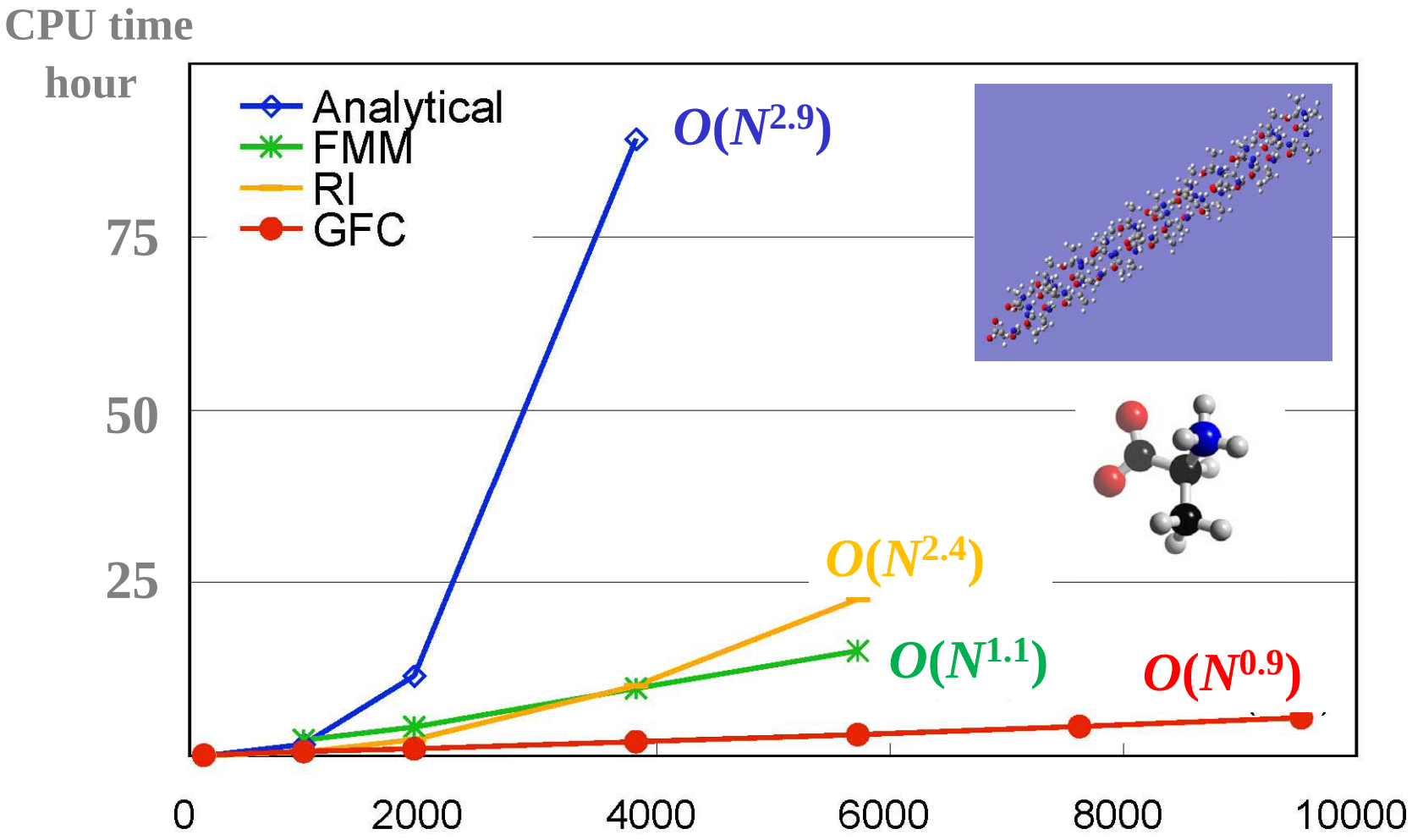
  *N*依存性を下げる理論、アルゴリズムの開発

- 電子密度法（密度汎関数法）

  簡潔で概念的、精度は汎関数に依存
  半定量的理論であり、大きな系に適用可能
  2次の分子物性、van der Waals力や励起状態の記述は悪い

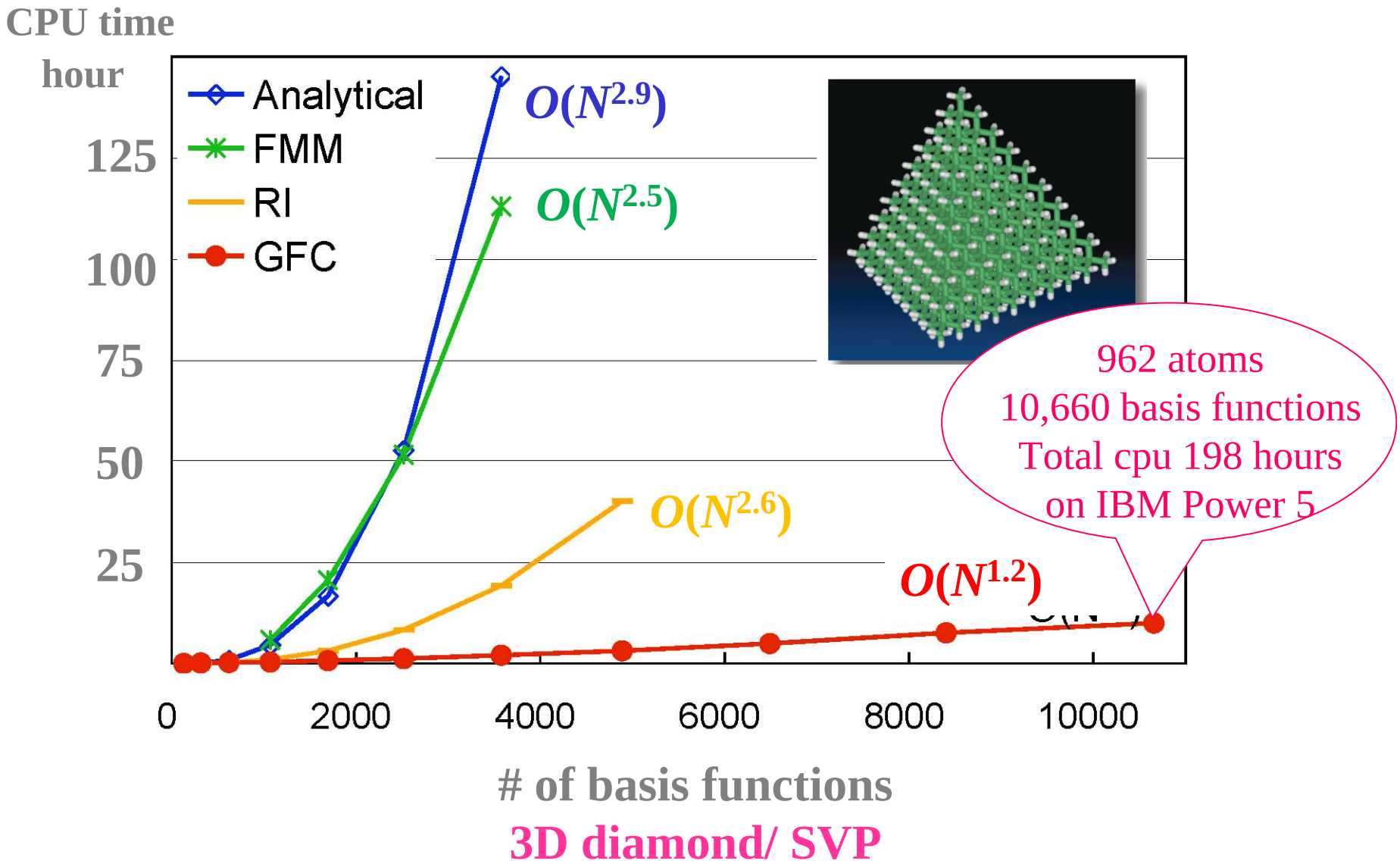
  より良い汎関数の開発

Gaussian and FE Coulomb Approach



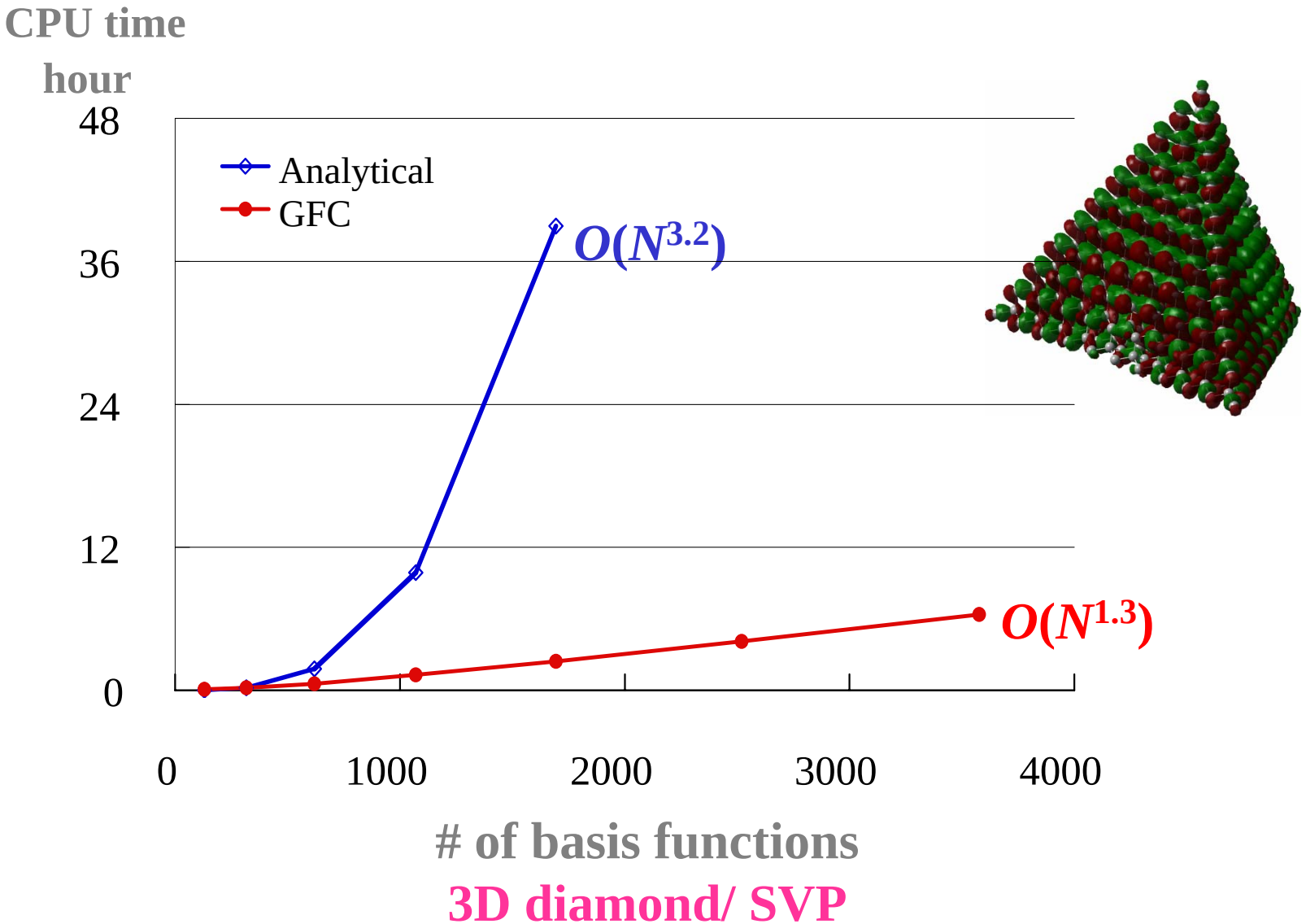
1D Alanine α-helix chain/ SVP

Gaussian and FE Coulomb Approach



3D diamond/ SVP

Energy Gradient
Gaussian and FE Coulomb Approach



3D diamond/ SVP

長距離補正の汎関数 (LC-DFT)

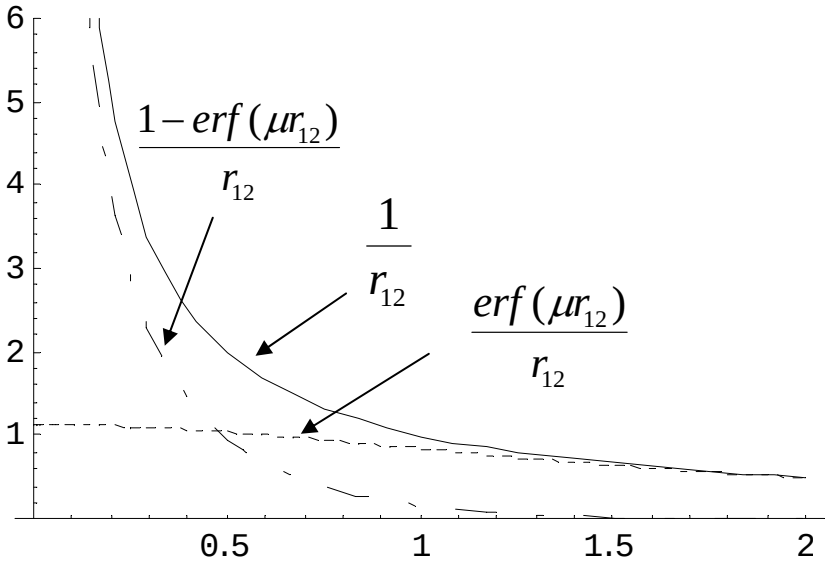
電子間反発 $1/r_{12}$ をEwald分割法を利用して長距離、短距離部分に分け、
短距離部はDFT汎関数、長距離部はHartree-Fock交換で表現

$$\frac{1}{r_{12}} = L(r_{12}) + \left(\frac{1}{r_{12}} - L(r_{12})\right) \qquad \left(L(r_{12}) = \frac{erf(\mu r_{12})}{r_{12}}, \quad \frac{erf(\mu r_{12})}{r_{12}} - \frac{2\mu}{\sqrt{\pi}} e^{-(1/a)\mu^2 r_{12}^2}, \cdots\right)$$

$$\frac{1}{r_{12}} = \frac{erf(\mu r_{12})}{r_{12}} + \frac{1-erf(\mu r_{12})}{r_{12}}$$

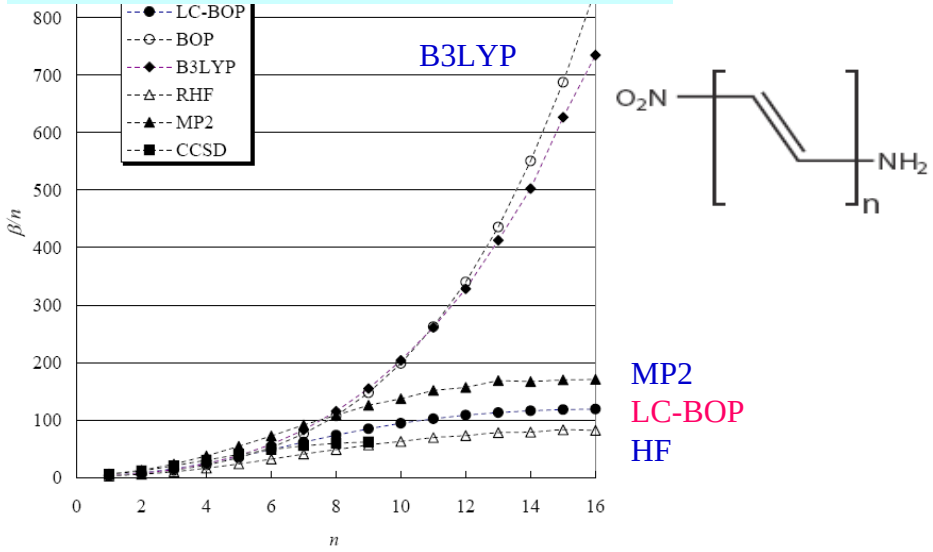
⇧ ⇧

HF exchange *GGA exchange*



2次の分子物性の改善

*Hyperpolarizability*の改善



励起エネルギー計算の平均誤差(eV)

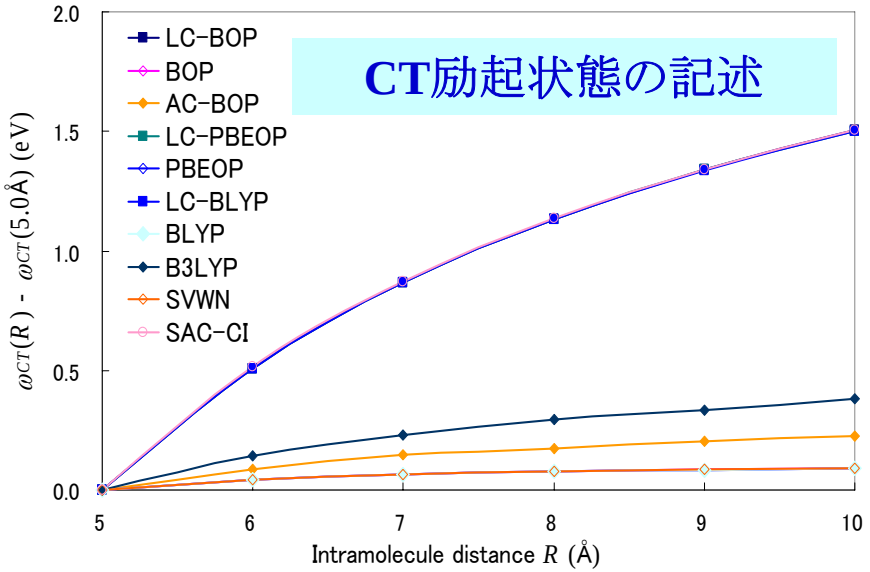
27 valence excitations (N_2, CO, H_2CO, C_2H_4, C_6H_6)

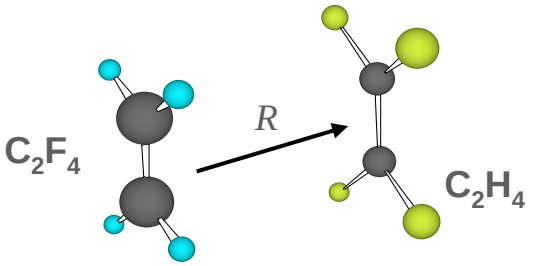
BLYP	0.36
B3LYP	0.37
LC-BLYP	0.32
SAC-CI	0.37

41 Rydberg excitations (N_2, CO, H_2CO, C_2H_4, C_6H_6)

BLYP	1.54
B3LYP	0.89
LC-BLYP	0.41
SAC-CI	0.19

CT励起状態の記述





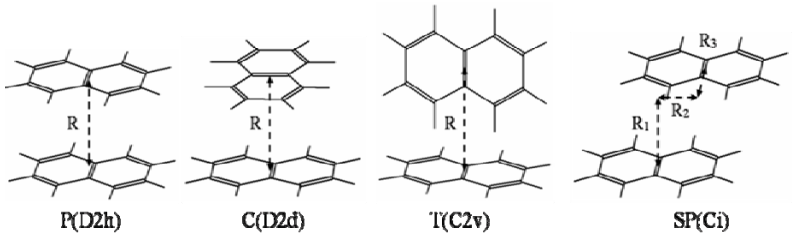
ΔE_{CT}(eV)

BLYP	5.40
B3LYP	7.49
LC-BLYP	12.49
Exptl.	12.5

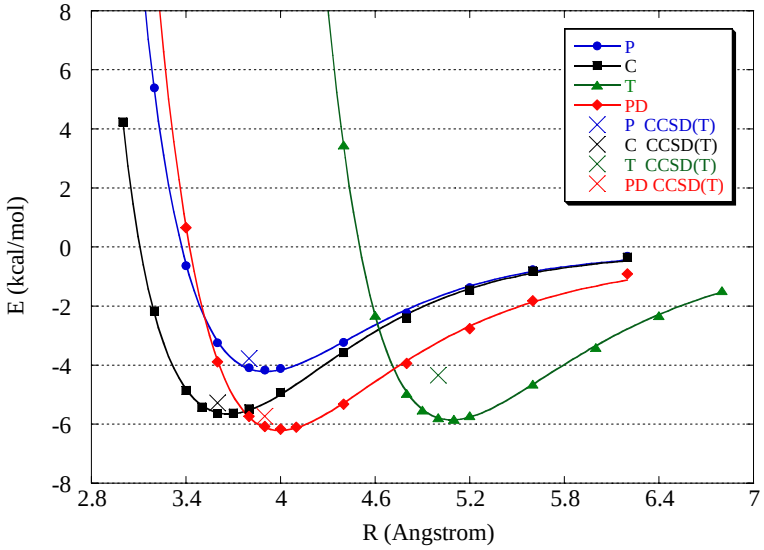
van der Waals分子の記述

Naphthalene Dimer

これまでのGGA汎関数はすべてrepulsive



Our DFT with *6-31+G***

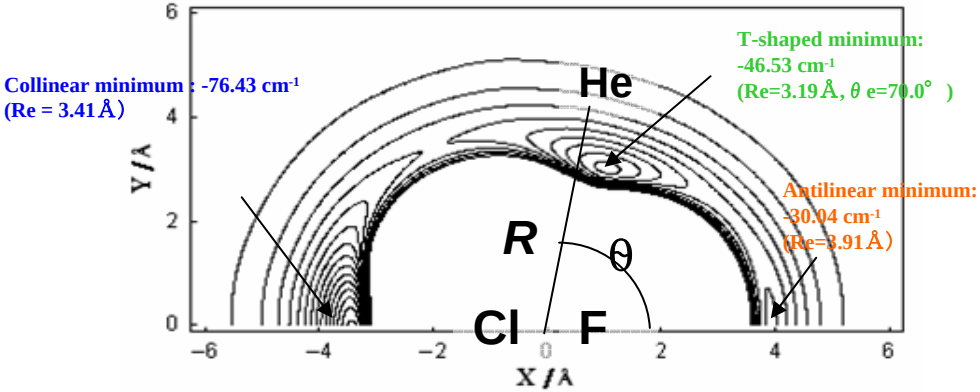


Our DFT 6.16 kcal/mol
CBS CCSD(T) 5.73 kcal/mol

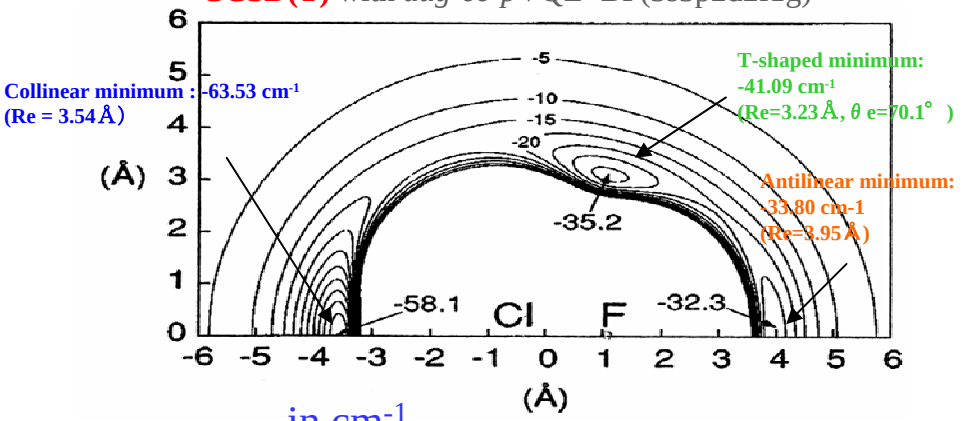
ClF…He

これまでの汎関数はLinear structuresのみを与える

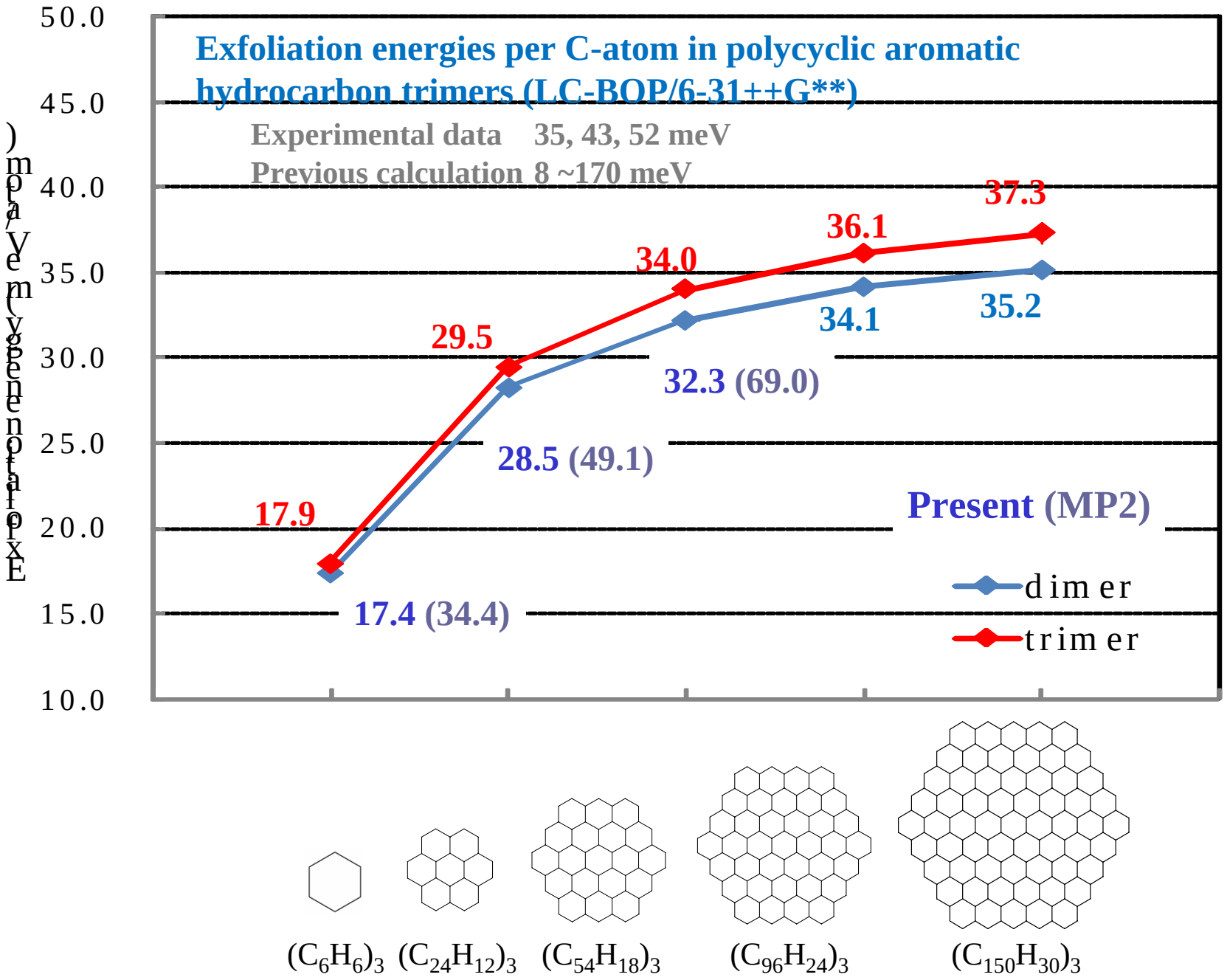
Our DFT with *aug-cc-p*VQZ



CCSD(T) with *aug-cc-p*VQZ+BF(3s3p2d2f1g)



in cm^{-1}


Exfoliation energies per C-atom in polycyclic aromatic hydrocarbon trimers (LC-BOP/6-31++G**)
Experimental data 35, 43, 52 meV
Previous calculation 8 ~170 meV
Present (MP2)
dimer
trimer
17.9
29.5
34.0
36.1
37.3
17.4 (34.4)
28.5 (49.1)
32.3 (69.0)
34.1
35.2
50.0
45.0
40.0
35.0
30.0
25.0
20.0
15.0
10.0
(C6H6)3
(C24H12)3
(C54H18)3
(C96H24)3
(C150H30)3

*UTChem*プロジェクト – 理論の実用化

理論化学のソフトウエアは物質科学の共通基盤
ソフトウエアの研究開発は欧米に大きく遅れをとる

世界の分子軌道プログラム・パッケージ

- DALTON
- Gaussian (Gaussian, Inc.)
- GAMESS (Iowa State Univ.
- Molpro
- Molcas (Lund Univ.)
- NWChem (PNNL)
- Q-Chem (Q-Chem, Inc.)

なぜ新しいソフトウェアが必要か

(1) 既存のプログラムを使うことで，多くの恩恵を受けてきた。しかし、プログラムの制限で真のブレークスルーは成し難い。
(2) 既存のプログラムでは取り扱うことができない重要で強力な方法論が多く存在する。

UTChem A Program Suite for ab initio Quantum Chemistry

Ab initio MO, DFT, and Dynamics

非相対論、相対論
（2成分、4成分相対論理論）

CISD, CISDT, CISDTQ,
CCSD, CCSDT, CCSDTQ,
MP2, MP3, and MP4,

パラレル版も用意

http://utchem.qcl.t.u-tokyo.ac.jp/

Conclusions

With the emergence of petascale computing platforms computational quantum chemistry is on the verge of entering a new era of modeling. It will enable us to tackle scientific problems that larger and more realistic than ever before, and to include more of the complex dynamical behavior of nature. Of course much more remains to be achieved but

Let's Do More Chemistry with Computers!