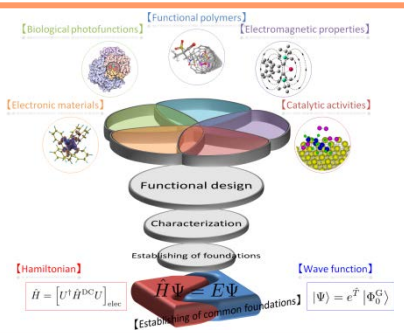
●FY2012　　Hiromi Nakai （Professor, Waseda University）

Theoretical Design of Materials with Innovative Functions Based on Relativistic Electronic Theory

Research Project Outline (From Oct. 2012 to Mar. 2018)

Clarification of the characters of elements that play primary roles and design of materials possessing innovative functions based on relativistic electronic theory.

◎To establish the relativistic quantum chemical methodology as a theoretical foundation.
◎To apply the method to catalytic activities, electromagnetic properties, electronic materials, biological photofunctions, and functional polymers.



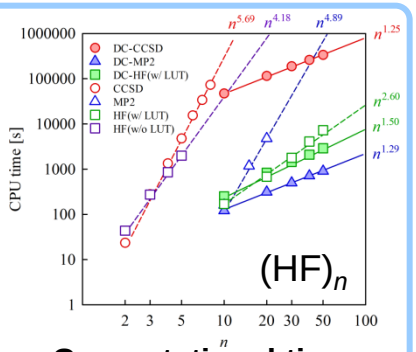
Research Results (FY2012)

◆Accurate and Efficient Relativistic Quantum Chemical Theory

✓ A scheme for highly accurate and efficient production of relativistic Hamiltonian was developed based on local unitary transformation and infinite-order Douglas-Kroll method.
✓ The extension to divide-and-conquer method realizes overall linear-scaling calculation.
✓ Largest molecular calculations including heavy atoms with highly accurate relativistic quantum chemistry were performed.

J. Chem. Phys. 139, 034109 (2013).

Scheme for accurate predictions in real system



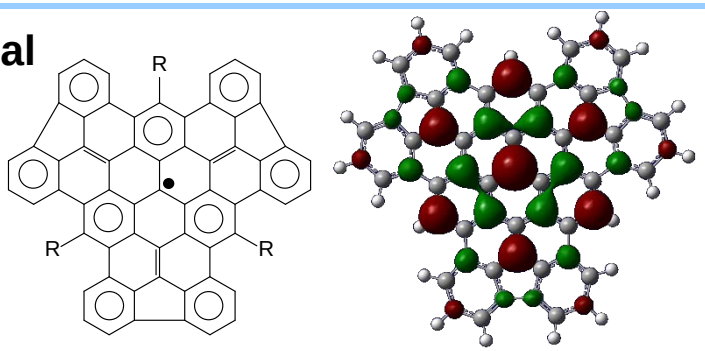
Computational time

◆Theoretical Design of Stable Hydrocarbon Radical

✓A novel hydrocabon radical “superphenalenyl was proposed based on trioxotriangulene (TOT).
✓Theoretical calculation of spin distribution and reaction energy predicted high stability.
✓High redox activity is expected as in the case of TOT.

Chem. Lett., 42, 1386 (2013).

Collaboration study with Morita team



Structural formula and SOMO of superphenalenyl