

6-2 理論・計算分子科学研究領域

理論分子科学第一研究部門

永 瀬 茂 (教授) (2001 年 4 月 1 日 ~ 2012 年 3 月 31 日)*)

A-1) 専門領域：理論化学，計算化学

A-2) 研究課題：

- a) 高周期元素の特性を利用した分子設計と反応
- b) 分子のサイズと形状を利用した分子設計と反応

A-3) 研究活動の概略と主な成果

- a) 高周期元素は新しい結合と多種多様な機能電子系の宝庫である。このために，高周期元素を骨格にもつ新規な化合物の構造，結合特性，電子特性，反応等を理論と計算および実験と共同して明らかにした。
- b) サイズの大きい分子が与える外部空間および内部空間は新しい機能発現として有用である。金属内包フラーレン，カーボンナノチューブ，ナノグラフェン等のナノカーボン系を取り上げて，化学修飾あるいはドーピングによる機能化と伝導性を理論と計算あるいは実験と共同して明らかにした。

B-1) 学術論文

H. KURIHARA, X. LU, Y. IIDUKA, H. NIKAWA, N. MIZOROGI, Z. SLANINA, T. TSUCHIYA, S. NAGASE and T. AKASAKA, “X-Ray Structures of $\text{Sc}_2\text{C}_2@\text{C}_{2n}$ ($n = 40, 41, 42$): In-Depth Understanding of the Core-Shell Interplay in Carbide Cluster Metallofullerenes,” *Inorg. Chem.* **51**, 746–750 (2012).

H. KURIHARA, X. LU, Y. IIDUKA, N. MIZOROGI, Z. SLANINA, T. TSUCHIYA, S. NAGASE and T. AKASAKA, “ $\text{Sc}_2@\text{C}_{3v}(8)\text{-C}_{82}$ vs. $\text{Sc}_2\text{C}_2@\text{C}_{3v}(8)\text{-C}_{82}$: Drastic Effect of C_2 Capture on the Redox Properties of Scandium Metallofullerenes,” *Chem. Commun.* **48**, 1290–1292 (2012).

S. SATO, H. NIKAWA, S. SEKI, L. WANG, G. LUO, J. LU, M. HARANAKA, T. TSUCHIYA, S. NAGASE and T. AKASAKA, “A Co-Crystal Composed of the Paramagnetic Endohedral Metallofullerene $\text{La}@\text{C}_{82}$ and a Nickel Porphyrin with High Electronic Mobility,” *Angew. Chem., Int. Ed.* **51**, 1589–1591 (2012).

H. KURIHARA, X. LU, Y. IIDUKA, H. NIKAWA, N. MIZOROGI, Z. SLANINA, T. TSUCHIYA, S. NAGASE and T. AKASAKA, “Chemical Understanding of Carbide Cluster Metallofullerenes: A Case Study on $\text{Sc}_2\text{C}_2@\text{C}_{2v}(5)\text{-C}_{80}$ with Complete X-Ray Crystallographic Characterizations,” *J. Am. Chem. Soc.* **134**, 3139–3144 (2012).

X. ZHAO, W. -Y. GAO, T. YANG, J. -J. ZHENG, L. -S. LI, L. HE, R. -J. GAO and S. NAGASE, “Violating the Isolated Pentagon Rule (IPR): Endohedral Non-IPR C_{98} Cages of $\text{Gd}_2@\text{C}_{98}$,” *Inorg. Chem.* **51**, 2039–2045 (2012).

H. -X. YEONG, S. -H. ZHANG, H. -W. XI, J. -D. GUO, K. H. LIM, S. NAGASE and C. -W. SO, “An Amidinate-Stabilized Germatrisilacyclobutadiene Ylide,” *Chem. -Eur. J.* **18**, 2685–2691 (2012).

- S. KARTHIKEYAN and S. NAGASE**, “Origins of the Stability of Imidazole–Imidazole, Benzene–Imidazole, and Benzene–Indole Dimers: CCSDS(T)/CBS and SAPT Calculations,” *J. Phys. Chem. A* **116**, 1694–1700 (2012).
- M. SAITO, Y. HASHIMOTO, T. TAJIMA, K. ISHIMURA, S. NAGASE and M. MINOURA**, “Molecular Structure of Dibenzo[*a,e*]pentalenen Anion Radical and its Electronic State,” *Chem. –Asian. J.* **7**, 480–483 (2012).
- Y. MAEDA, M. YAMADA, T. HASEGAWA, T. AKASAKA, J. LUO and S. NAGASE**, “Interaction of Single-Walled Carbon Nanotubes with Amine,” *NANO* **7**, 1130001 (10 pages) (2012).
- H. KURIHARA, Y. IIDUKA, Y. RUBIN, M. WAELECHLI, N. MIZOROGI, Z. SLANINA, T. TSUCHIYA, S. NAGASE and T. AKASAKA**, “Unexpected Formation of a $\text{Sc}_3\text{C}_2@\text{C}_{80}$ Bisfulleroid Derivative,” *J. Am. Chem. Soc.* **134**, 4092–4095 (2012).
- T. AGOU, Y. SUGIYAMA, T. SASAMORI, H. SAKAI, Y. FURUKAWA, N. TAKAGI, J. -D. GUO, S. NAGASE, D. HASHIZUME and N. TOKITOH**, “Synthesis of Kinetically Stabilized 1,2-Dihydorodisilenes,” *J. Am. Chem. Soc.* **134**, 4120–4123 (2012).
- X. LU, T. AKASAKA and S. NAGASE**, “Soluble and Tubular Higher Fullerenes that Encapsulate Metals,” *Angew. Chem., Int. Ed.* **51**, 2812–2814 (2012).
- R. QUHE, J. ZHENG, G. LUO, Q. LIU, R. QIN, J. ZHOU, D. YU, S. NAGASE, W. -N. MEI, Z. GAO and J. LU**, “Tunable and Sizable Band Gap of Single Layer Graphene Sandwiched between Hexagonal Boron Nitride,” *NPG Asia Materials* **4**, e6 (10 pages) (2012).
- N. KANO, A. FURUTA, T. KANBE, J. YOSHINO, Y. SHIBATA, T. KAWASHIMA, N. MIZOROGI and S. NAGASE**, “2,2’-Diborylazobenzenes with Double N–B Coordination: Control of Fluorescent Properties by Substituents and Redox Reactions,” *Eur. J. Inorg. Chem.* 1584–1587 (2012).
- C. A. CAPUTO, J. -D. GUO, S. NAGASE, J. C. FETTINGER and P. P. POWER**, “Reversible and Irreversible Higher-Order Cycloaddition Reactions of Polyolefins with a Multiple-Bonded Heavier Group 13 Alkene Analogue: Contrasting the Behavior of Systems with π – π , π – π^* and π – π^+ Frontier Molecular Orbital Symmetry,” *J. Am. Chem. Soc.* **134**, 7155–7164 (2012).
- M. SUZUKI, X. LU, S. SATO, H. NIKAWA, N. MIZOROGI, Z. SLANINA, T. TSUCHIYA, S. NAGASE and T. AKASAKA**, “Where Does the Metal Cation Stay in $\text{Gd}@C_{2v}(9)\text{-C}_{82}$? A Single-Crystal X-Ray Diffraction Study,” *Inorg. Chem.* **51**, 5270–5273 (2012).
- C. XU, G. LUO, Q. LIU, J. ZHENG, Z. ZHANG, S. NAGASE, Z. GAO and J. LU**, “Giant Magnetoresistance in Silicene Nanoribbons,” *Nanoscale* **4**, 3111–3117 (2012).
- Z. D. BROWN, J. -D. GUO, S. NAGASE and P. P. POWER**, “Experimental and Computational Study of Auxiliary Molecular Effects on the Mechanism of the Addition of Hydrazines to a Low-Valent Germanium Complex,” *Organometallics* **31**, 3768–3772 (2012).
- X. LU, K. NAKAJIMA, Y. IIDUKA, H. NIKAWA, T. TSUCHIYA, N. MIZOROGI, Z. SLANINA, S. NAGASE and T. AKASAKA**, “The Long-Believed $\text{Sc}_2@\text{C}_{2v}(17)\text{-C}_{84}$ is Actually $\text{Sc}_2\text{C}_2@\text{C}_{2v}(9)\text{-C}_{82}$: Unambiguous Structure Assignment and Chemical Functionalization,” *Angew. Chem., Int. Ed.* **51**, 5889–5892 (2012).
- Q. ZHENG, G. LUO, Q. LIU, R. QUHE, J. ZHENG, K. TANG, Z. GAO, S. NAGASE and J. LU**, “Structural and Electronic Properties of Bilayer and Trilayer Graphdiyne,” *Nanoscale* **4**, 3990–3996 (2012).

B-3) 総説, 著書

永瀬 茂, 「大きい分子の量子化学計算——多重結合分子と金属内包フラーレンを例として」CSJ カレントレビュー 08 「巨大分子系の計算化学——超大型計算機時代の理論化学の新展開」日本化学会篇, 化学同人, 100–105 (2012).

Z. SLANINA, F. UHLIK, S. -L. LEE, T. AKASAKA and S. NAGASE, “Stability Computation for Fullerenes and Metallofullenes,” in *Handbook of Carbon Nano Materials*, F. D’Souza and K. M. Kadish, Eds., World Scientific, **Vol. 4**, pp. 381–429 (2012).

Y. MAEDA, T. AKASAK and S. NAGASE, “Endohedral Metallofullerene Functionalization,” in *Advances in Carbon Nanomaterials: Science and Applications*, N. Tagmatarchis Ed., Pan Stanford Publishing, pp. 269–298 (2012).

B-4) 招待講演

永瀬 茂, 「実験とのインタープレイ」第22回神奈川大学シンポジウム(計算化学最前線)平塚, 2012年3月.

*) 2012 年 3 月 31 日退職

2012 年 4 月 1 日京都大学福井謙一記念研究センターシニアリサーチフェロー