平成２８年度報告書

研究代表者氏名：吉澤　一成、研究項目：A04
研究分担者氏名：　塩田　淑仁

【研究課題名】
酵素触媒反応種の状態変化と活性制御に関する理論的研究

【各研究項目の連携状況】
領域内の他の研究グループとの連携状況（予定を含む）について、①簡略化した共同研究内容②連携研究代表者姓（研究項目班）③共著論文の有無（件数）を研究内容毎に記載

1. ①量子化学計算による金属錯体の反応解析、②小島隆彦（A04)、③有（4）
2. ①量子化学計算による金属錯体の反応解析、②小澤文幸（A03)、③有（2）
3. ①量子化学計算による金属錯体の反応解析、②杉本秀樹（A04)、③有（1）
4. ①量子化学計算による金属錯体の電子状態解析、②石森浩一郎（A04)、③有（1),
5. ①量子化学計算による金属錯体の電子状態解析、②林　高史（A04)、③有（3),
6. ①量子化学計算による有機化合物の反応解析、②安倍　学（A02)、③有（1）
7. ①量子化学計算による金属錯体の電子状態解析、②金川慎治（A04)、③有（4),

【原著論文】

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【総説・解説】

1 樋口千紗, 吉澤一成*, 炭素とエポキシ樹脂の接着に関する量子力学的接着理論, 機能材料, 36(6), 9-16 (2016).
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【新聞等の媒体掲載, 学術雑誌表紙掲載等】

2016.8.1:「窒素活性化」に関する研究が, 日経新聞に掲載

大気中の窒素
触媒でアンモニアに
東大・九大、手軽に合成

東京大学の西林仁昭教授と九州大学の吉沢一成教授らは、大気中の窒素を燃料や肥料に使うアンモニアに変える触媒を開発した。鉄を含む化合物で、一部の植物が窒素分からアンモニアを合成するときに使う酵素の構造をまねた。溶剤に溶かしてアンモニアを手軽に合成できるという。従来の合成法は超高温・超高圧が必要だった。燃料電池車の燃料などへ応用を目指す。

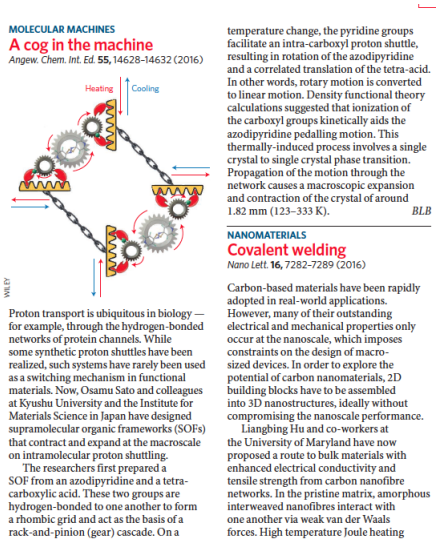
現在、アンモニアはハーバー・ボッシュ法と呼ぶ技術を使い、化石燃料から作る水素と窒素を400～600度、数百気圧で反応させ作る。

研究チームは、マメ科植物の根に住む根粒菌が大気中の窒素と水の水素イオンからアンモニアを合成するのに使う酵素に着目した。酵素の構造を鉄を含む化合物で再現したところ、電子と水素イオンを発生させる試薬のもとで、大気中の窒素からアンモニアができた。

今後は触媒が水に溶け、試薬が無くてもアンモニアを発生するように改良する。詳細な内容を英科学誌ネイチャー・コミュニケーションズ（電子版）に掲載した。

2016.8.30：「窒素活性化」に関する研究が，Angew. Chem. Int. Ed., 55, 1 (2016).に掲載（表紙）

(2016.12.12)：「分子機械(A cog in the machine)」に関する研究が Nature Nanotechnology の research highlights に掲載



MOLECULAR MACHINES

A cog in the machine

Angew. Chem. Int. Ed. **55,** 14628–14632 (2016)

Proton transport is ubiquitous in biology — for example, through the hydrogen-bonded networks of protein channels. While some synthetic proton shuttles have been realized, such systems have rarely been used as a switching mechanism in functional materials. Now, Osamu Sato and colleagues at Kyushu University and the Institute for Materials Science in Japan have designed supramolecular organic frameworks (SOFs) that contract and expand at the macroscale on intramolecular proton shuttling.

The researchers first prepared a SOF from an azodipyridine and a tetra-carboxylic acid. These two groups are hydrogen-bonded to one another to form a rhombic grid and act as the basis of a rack-and-pinion (gear) cascade. On a temperature change, the pyridine groups facilitate an intra-carboxyl proton shuttle, resulting in rotation of the azodipyridine and a correlated translation of the tetra-acid. In other words, rotary motion is converted to linear motion. Density functional theory calculations suggested that ionization of the carboxyl groups kinetically aids the azodipyridine pedalling motion. This thermally-induced process involves a single crystal to single crystal phase transition. Propagation of the motion through the network causes a macroscopic expansion and contraction of the crystal of around 1.82 mm (123–333 K). *BLB*

NANOMATERIALS

Covalent welding

Nano Lett. **16,** 7282–7289 (2016)

Carbon-based materials have been rapidly adopted in real-world applications. However, many of their outstanding electrical and mechanical properties only occur at the nanoscale, which imposes constraints on the design of macro-sized devices. In order to explore the potential of carbon nanomaterials, 2D building blocks have to be assembled into 3D nanostructures, ideally without compromising the nanoscale performance.

Liangbing Hu and co-workers at the University of Maryland have now proposed a route to bulk materials with enhanced electrical conductivity and tensile strength from carbon nanofibre networks. In the pristine matrix, amorphous interweaved nanofibres interact with one another via weak van der Waals forces. High temperature Joule heating

【受賞について】

(研究代表者の受賞)

2017.2.13：吉澤一成，BCSJ 賞受賞

“σ -CAM Mechanisms for the Hydrogenation of Alkenes by cis- and trans-Disilametallacyclic Carbonyl Complexes (M = Fe, Ru, Os): Experimental and Theoretical Studies”

（研究協力者の受賞）

2016.1.27：辻雄太（助教），第 1 回福井謙一奨励賞受賞

“理論化学研究に立脚した量子干渉現象の分子エレクトロニクスへの展開”

【若手研究者間の取り組みについて】

2016.7.12：若手研究者で「ケモインフォマティクスに関する」研究会を実施した.

2016.2.1~3.1：若手研究者で Li Jun 博士を招き研究交流を実施した.

【新学術に関連したシンポジウムや研究会などの開催状況】

2016.4.17~21：「藤原セミナー」（福岡）

【アウトリーチの実施状況】

2016.8.1：藤原セミナーで実施した支援活動が熊本日日新聞に掲載

熊本日日新聞

支援の輪

海外研究者も義援金

ノーベル化学賞 ホフマン博士ら 宇城市に贈る

2016.8.6：九州大学オープンキャンパスに出展