生命分子システムにおける
動的秩序形成と高次機能発現

領域番号　2501

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新学術領域研究（研究領域提案型）研究成果報告書

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はしがき

本研究成果報告書は、平成 25 年度から 29 年度の期間において、科学研究費補助金新学術領域研究（研究領域提案型）により行われた「生命分子システムにおける動的秩序形成と高次機能発現」（領域番号 2501）に関する成果をまとめたものである。

生命現象の特徴は、複雑な柔構造を有する多様な生命分子素子が動的な集合体を形成することにより、自律的に秩序あるシステムを創出することにある。こうしたシステムの形成原理を解明することは生命現象の本質的理解につながるはずである。本研究領域は、生命分子システムを構成する多数の素子がダイナミックな離合集散を通じて動的秩序を形成し、それが時間発展して高次機能を発現する仕組みを分子科学の観点から解き明かすことを目指す。そのために物理化学に基盤をおく実験と理論の融合研究を展開する。さらに、生命分子科学と超分子化学のアプローチを発展的に統合することによって、生命分子システムの特質を具現化した動的秩序系を人工的に構築することを目指す。この目的を実現するために、生命分子科学を基軸に、生物物理学、理論・計算科学、合成化学、構造・システム生物学、さらには医学・薬学・工学・環境科学等への応用を見据えた研究ネットワークを組織する。こうした国際的にも類例のない学際的な研究体制を構築することにより、生命の本質的理解に向けた先端的な学術領域を創成する。その成果は、創薬をはじめとする産業応用の進展に資するとともに、生命科学一般の深化と分子科学におけるパラダイムシフトをもたらし、人工的な生命システムを設計・創生するための指導原理を導き出すことが期待される。

本研究領域では、動的秩序の探査（A01）・創生（A02）・展開（A03）の３つの研究項目を研究の柱とし、各項目内において化学・物理学・生物学の分野横断的研究を実施するとともに、これらの研究項目の枠組みを越えた共同研究を活発に行なって順調に成果を上げることができた。A01 と A02 の連携により、人工錯体の分子集合過程で生じる過渡的化学種を実験的に観測する方法を開発し、それらの遷移ダイナミクスの全容を捉える独創的な分子理論を打ち立てることに成功した。A03 の研究で初めて明らかとなった生体超分子の形成機構とあわせて、人工分子系と生命分子系に底通する自己集合の原理を浮き彫りにすることができた。さらに、アミロイド線維や時計タンパク質などを対象に、非平衡系における生体分子の離合集散過程について、実験と理論の両面から詳細に解き明し、それらの特質を備えた人工分子系の創生も実現している(A01、A02、A03 の連携)。特に、分子集合のエネルギーランドスケープにおける速度論支配と熱力学支配を制御することで超分子形成の時間発展のプログラミングが可能となり、同調的に周期的律動をする人工高分子ゲルや生体分子と人工超分子のハイブリッド化による高次機能の創出にも成果をおさめている。成果発信はもとより、若手育成と国際連携も成功裡に達成することができた。このように、本研究領域の活動を通じて、人工分子系と生命分子系を貫く動的秩序形成機構の普遍性が初めて見出され、人工的な生命システムを創生する指針を導き出すことができた。

研究組織

（総：総括班，支：国際活動支援班，計：総括班及び国際活動支援班以外の計画研究，公：公募研究）

【計画研究】

研究項目	課題番号 研究課題名	代表者氏名	所属機関 部局 職	研究分担者・研究連携者（研究者番号）
X00 総	25102001 生命分子システムにおける動的秩序形成と高次機能発現の研究に関する総括	加藤　晃一	自然科学研究機構・岡崎統合バイオサイエンスセンター・教授	佐藤啓文 上久保裕生 寺嶋正秀 平岡秀一 芳坂貴弘 佐藤宗太 岡本祐幸 稲垣直之 （いずれも計画班員）
Y00 支	15K21708 生命分子システムにおける動的秩序形成と高次機能発現の研究推進のための国際活動支援	加藤　晃一	自然科学研究機構・岡崎統合バイオサイエンスセンター・教授	佐藤啓文 上久保裕生 寺嶋正秀 平岡秀一 芳坂貴弘 佐藤宗太 岡本祐幸 稲垣直之 （いずれも計画班員）
A01 計	25102002 分子集積と秩序形成の分子理論	佐藤　啓文	京都大学・大学院工学研究科・教授	山本武志 (30397583)
A01 計	25102003 機能を生み出す単位生体分子集団（機能モジュール）の動的秩序の探査	上久保　裕生	奈良先端科学技術大学院大学・物質創成科学研究科・教授	片岡幹雄 (30150254)
A01 計	25102004 動的秩序・崩壊のダイナミクスから観る高次機能発現の分子機構解明	寺嶋　正秀	京都大学・大学院理学研究科・教授	
A02 計	25102005 分子表面の精密デザインに基づく人工系における自己組織化制御	平岡　秀一	東京大学・大学院総合文化研究科・教授	
A02 計	25102006 生命分子システムの有機化学的拡張による動的秩序の創出	芳坂　貴弘	北陸先端科学技術大学院大学・マテリアルサイエンス研究科・教授	
A02 計	25102007 生体分子系を模倣した動的秩序をもつ人工分子の開発	佐藤　宗太	東京大学・大学院理学系研究科（理学部）・准教授	
A03 計	25102008 生命分子の動的秩序形成におけるミクロ－マクロ相関の探査と設計原理の探求	加藤　晃一	自然科学研究機構・岡崎統合バイオサイエンスセンター・教授	山口拓実 (60522430) 佐藤匡史 (80532100) 栗原顕輔 (80740919) 矢木真穂 (40608999) 谷中冴子 (80722777)

A03 計	25102009 生体分子集団および人工分子集団の相互作用と大規模構造転換	岡本　祐幸	名古屋大学・大学院理学研究科・教授	
A03 計	25102010 生体分子素子の自己組織化による細胞の動的秩序形成	稲垣　直之	奈良先端科学技術大学院大学・バイオサイエンス研究科・教授	

【公募研究】

平成 26 年度～27 年度

研究項目	課題番号 研究課題名	代表者氏名	所属機関 部局 職	研究分担者・研究連携者（研究者番号）
A01 公	26102501 膜孔形成毒素の動的な作用機構の解明	田中　良和	北海道大学・大学院先端生命科学研究科（研究院）・准教授	
A01 公	26102511 ｓＨｓｐの動的秩序制御による機能発現の分子機構解明	養王田　正文	東京農工大学・大学院工学研究院・教授	
A01 公	26102512 トポロジー変換可能な新規超分子ポリマーの合成と組織化・機能制御	高田　十志和	東京工業大学・大学院理工学研究科・教授	
A01 公	26102514 ヒトカルシトニンのアミロイド線維形成および阻害の分子機構の解明	内藤　晶	横浜国立大学・大学院工学研究院・教授	川村 出 (20452047)
A01 公	26102515 高速ＡＦＭを用いたＫａｉタンパク質の複合体形成過程のダイナミクス観察	内橋　貴之	金沢大学･数物科学系･教授	
A01 公	26102525（廃止） キュミュラント粗視化動力学によるタンパク質動的秩序形成過程の理論研究	重田　育照	筑波大学・大学院数理物質科学研究科・教授	
A01 公	26102526 細菌の細胞分裂ダイナミクスの構造機能相関解析	松村　浩由	立命館大学･生命科学部･教授	
A01 公	26102527 脂質ラフトにおける脂質分子の動的秩序解析	松森　信明	九州大学・大学院理学研究院・教授	木下祥尚 (40529517)
A02 公	26102532（廃止） タンパク質分泌システムの精密探査を可能とする新しい再構成系の構築	塚崎　智也	奈良先端科学技術大学院大学・バイオサイエンス研究科・准教授	
A01 公	26102533 多価カチオンによって媒介される酸性蛋白質間引力の制御と動的秩序構造	秋山　良	九州大学・大学院理学研究院・准教授	
A01 公	26102534 超分子複合系ソフトマターの秩序構造とダイナミクス	安中　雅彦	九州大学・大学院理学研究院・教授	
A01 公	26102538 生細胞内の秩序構造が誘起する蛋白質立体構造の安定性	池谷　鉄兵	首都大学東京・理工学研究科・助教	伊藤隆 (80261147) Peter Güntert (首都大学東京・理工学研究科・客員教授)

A01 公	26102539 量子シミュレーション手法の深化による超分子および生体分子の自己集合機構の解明	立川　仁典	横浜市立大学・大学院生命ナノシステム科学研究科・教授	
A01 公	26102541 人工脂質二重膜におけるドメイン構造の実験的探究	岩田　耕一	学習院大学･理学部･教授	
A02 公	26102542（廃止） 動的秩序を示すバイオインスパイアードⅱ電子系ーイオン複合体の創製	前田　大光	立命館大学･薬学部･教授	
A01 公	26102544 Ｘ線小角散乱と液中高速ＡＦＭの相補利用による分子時計の離合集散計測	秋山　修志	分子科学研究所・協奏分子システム研究センター・教授	内橋貴之 (30326300) 向山厚 (80647446)
A02 公	26102502 動的秩序形成を利用した化学反応応答システムの開発	佐田　和己	北海道大学・大学院理学研究院・教授	
A02 公	26102504 コート小胞形成における動的秩序形成メカニズムの解明	二井　勇人	東北大学・大学院農学研究科・准教授	
A02 公	26102507 ＡＴＰ駆動サイボーグ回転分子モーターの創生	飯野　亮太	自然科学研究機構・岡崎統合バイオサイエンスセンター・教授	
A02 公	26102508 ペプチドフォールディングと超分子錯体によるハイブリッド動的秩序形成	澤田　知久	東京大学・大学院工学系研究科・助教	
A02 公	26102513 人工分子針の細胞膜貫通制御	上野　隆史	東京工業大学・大学院生命理工学研究科・教授	
A02 公	26102517 高分子コロイド分散系における動的秩序の構築	鈴木　大介	信州大学･繊維学部･准教授	
A02 公	26102518 ＤＮＡを相互作用素子として細胞様運動する人工システムの構築	神谷　由紀子	名古屋大学・エコトピア科学研究所・講師	
A02 公	26102522 生体膜における曲率形成と膜の形態変化を誘導・制御するペプチドツール	二木　史朗	京都大学･化学研究所･教授	河野健一 (70732874)
A02 公	26102528 リポソーム内膜タンパク質合成系を用いた細胞膜動態の再構成	松浦　友亮	大阪大学・大学院工学研究科・准教授	
A02 公	26102540 メタロペプチドの分子認識化学を活用した動的秩序の多段階創生とタイムプログラミング	三宅　弘之	大阪市立大学・大学院理学研究科・准教授	
A02 公	26102546 感染性の超分子集合体：メカニズムの解明および時間発展の分子論的制御	杉安　和憲	国立研究開発法人物質・材料研究機構・分子機能化学グループ・主任研究員	
A03 公	26102505 アクチン骨格超分子集合体の動的秩序形成機構と細胞遊走、力覚応答における機能	水野　健作	東北大学・大学院生命科学研究科・教授	
A03 公	26102509 細胞内輸送小胞の形成を支える動的秩序の解明	佐藤　健	東京大学・大学院総合文化研究科・准教授	

A03 公	26102510 鞭毛の振動運動発現に至る動的秩序形成	真行寺　千佳子	東京大学・大学院理学系研究科・准教授	
A03 公	26102516 チャネル蛋白質の構造変化に連携した自己組織化動態：チャネル新規機能発現機構の解明	老木　成稔	福井大学・医学部・教授	
A03 公	26102520 タンパク質物性から振動の理論生物学へ	笹井　理生	名古屋大学・大学院工学研究科・教授	
A03 公	26102524 生体分子集合体が形成する動的平衡の中性子小角散乱による研究	杉山　正明	京都大学・原子炉実験所・教授	
A03 公	26102529 生命分子機能を、時空間を制御して解明する設計分子プローブ	菊地　和也	大阪大学・大学院工学研究科・教授	堀雄一郎 (00444563) 蓑島維文 (20600844)
A03 公	26102530 質量分析による蛋白質複合体形成動的メカニズムの解明	内山　進	大阪大学・大学院工学研究科・准教授	石井健太郎 (30748380) 野田勝紀 (大阪大学・大学院工学研究科・特任研究員)
A03 公	26102531 アミロイド伝播核生成相におけるタンパク質分子の集合・秩序化メカニズムの解明	茶谷　絵理	神戸大学・大学院理学研究科・准教授	山本直樹 (90580671)
A03 公	26102543 時計タンパク質の解離集合による時間自動補正メカニズム	寺内　一姫	立命館大学・生命科学部・准教授	
A03 公	26102545 ロタウイルスの感染と増殖における構造秩序形成の解析	村田　和義	生理学研究所・脳機能計測・支援センター・准教授	片山和彦 (60342903)
A03 公	26102547 細胞膜受容体の動的会合体形成と分子認識反応	佐甲　靖志	国立研究開発法人理化学研究所・佐甲細胞情報研究室・主任研究員	
A03 公	26102550 親水性／疎水性溶液界面でのアミロイドベータペプチド凝集機構の理論的研究	奥村　久士	自然科学研究機構・計算科学研究センター・准教授	伊藤暁 (90595381) 森義治 (90646928)

平成 28 年度～平成 29 年度

研究 項目	課題番号 研究課題名	代表者氏名	所属機関 部局 職	研究分担者・研究連携者（研究者番号）
A01 公	16H00753 プレフォルディンー２型シャペロニンシステムのダイナミクスとフォールディング機構	養王田　正文	東京農工大学・大学院工学研究院・教授	篠原恭介 (20527387)
A01 公	16H00754 ロタキサン連結高分子系超分子における組織化制御	高田　十志和	東京工業大学・大学院理工学研究科・教授	青木大輔 (80736950)
A01 公	16H00756 脂質膜環境でのカルシトニンおよびグルカゴンのアミロイド線維形成分子機構の解明	内藤　晶	横浜国立大学・大学院工学研究院・名誉教授	川村 出 (20452047)

A01 公	16H00758 高速ＡＦＭ計測によるＫａｉタンパク質のロバストな概日周期発生機構の解明	内橋　貴之	名古屋大学・理学研究科・教授	
A01 公	16H00773 蛍光標識脂質を用いた脂質膜の動的秩序解析	松森　信明	九州大学・大学院理学研究院・教授	木下祥尚 (40529517)
A01 公	16H00774 多価カチオン媒介型実効引力に注目した蛋白質溶液の相挙動と動的秩序構造制御機構	秋山　良	九州大学・大学院理学研究院・准教授	
A01 公	16H00778 光捕集複合体における自己組織化過程と機能発現の理論的究明	東　雅大	琉球大学・理学部・助教	斉藤真司 (70262847)
A01 公	16H00779 生細胞内の秩序と蛋白質構造安定性の解明に向けた基盤技術	池谷　鉄兵	首都大学東京・理工学研究科・助教	伊藤隆 (80261147) Peter Güntert (首都大学東京・理工学研究科・客員教授)
A01 公	16H00780 超分子・生体分子の自己集合機構の理解のための量子シミュレーション手法の高度化	立川　仁典	横浜市立大学・大学院生命ナノシステム科学研究科・教授	
A01 公	16H00782 人工脂質二重膜におけるドメイン構造の実験的探求	岩田　耕一	学習院大学・理学部・教授	髙屋智久 (70466796)
A01 公	16H00783 細胞分裂の階層構造ダイナミクスの解明	松村　浩由	立命館大学・生命科学部・教授	内橋貴之 (30326300) 重田育照 (80376483)
A01 公	16H00785 Ｘ線溶液散乱と高速ＡＦＭを用いた生物時計因子の動的構造解析	秋山　修志	分子科学研究所・協奏分子システム研究センター・教授	内橋貴之 (30326300) 向山厚 (80647446)
A02 公	16H00755 Ｔ４ファージ由来蛋白質針による生体膜透過の動的秩序機構	上野　隆史	東京工業大学・大学院生命理工学研究科・教授	内橋貴之 (30326300) 古田忠臣 (10431834) 川野竜司 (90401702)
A02 公	16H00757 人工的なＤＮＡ類似体を基質とする核酸関連酵素反応の解析とその化学的深化	井上　将彦	富山大学・大学院医学薬学教育部（薬学系）・薬学部・教授	阿部肇 (10324055) 千葉順哉 (50436789)
A02 公	16H00760 高分子コロイド分散系における動的秩序の発展	鈴木　大介	信州大学・繊維学部・准教授	
A02 公	16H00761 人工蛋白質ナノブロック自己組織化超分子複合体の構造機能解析と動的秩序系設計構築	新井　亮一	信州大学・繊維学部・准教授	
A02 公	16H00762 人工核酸により発動する細胞様機能の構築	神谷　由紀子	名古屋大学・工学研究科・准教授	
A02 公	16H00763 生体膜における曲率形成と膜の形態変化を誘導・制御するペプチドツール	二木　史朗	京都大学・化学研究所・教授	河野健一 (70732874)
A02 公	16H00767 リポソーム内膜タンパク質発現系の発現ダイナミクス制御技術の確立と応用	松浦　友亮	大阪大学・大学院工学研究科・准教授	

A02 公	16H00775 複製開始蛋白質　ＤｎａＡに対する制御系の自律的連動システムの創生と動態原理の解析	片山　勉	九州大学･薬学研究院･教授	加生和寿 (90726019) 川上広宣 (50403952)
A02 公	16H00777 配位結合を利用した脂質膜上での動的秩序形成と機能発現	大谷　亮	熊本大学・自然科学研究科・助教	速水真也 (30321912)
A02 公	16H00781 動的ペプチド金属錯体からなる超分子集合体の秩序創生と動的変換プログラミング	三宅　弘之	大阪市立大学・大学院理学研究科・准教授	
A02 公	16H00787 分化する超分子集合体：エネルギーランドスケープに基づく高次構造と機能の制御	杉安　和憲	国立研究開発法人物質・材料研究機構・分子機能化学グループ・主任研究員	
A02 公	16H00789 糖質加水分解サイボーグリニア分子モーターの創生	飯野　亮太	自然科学研究機構・岡崎統合バイオサイエンスセンター・教授	
A03 公	16H00748 構造情報に基づいた機能変換による膜孔形成毒素の会合機構の解明	田中　良和	東北大学・生命科学研究科・教授	姚閔 (40311518) 加藤公児 (30452428)
A03 公	16H00749 アクチン骨格超分子集合体の動的秩序形成機構と細胞機能発現機構	水野　健作	東北大学・大学院生命科学研究科・教授	
A03 公	16H00752 鞭毛の振動運動発現に至るダイニンの自律的複雑性の時空間的展開	真行寺 千佳子	東京大学・大学院理学系研究科・准教授	
A03 公	16H00759 チャネル蛋白質のゲーティングに連動した離合集散動態の分子機構の解明	老木　成稔	福井大学・医学部・教授	
A03 公	16H00764 Ｐ４－ＡＴＰａｓｅによる生体膜のリン脂質動的秩序の形成機構	申　惠媛	京都大学･薬学研究科･准教授	
A03 公	16H00765 微生物集団が示す特異な動的秩序形成機構の解明とその制御	山本　量一	京都大学･工学系研究科･教授	John Jairo Molina (京都大学・工学研究科・助教)
A03 公	16H00766 巨大タンパク質会合体における動的ネットワークとその機能解明	杉山　正明	京都大学･原子炉実験所･教授	内山進 (90335381) 長田裕也 (60512762)
A03 公	16H00768 生命分子機能を、時空間を制御して解明する設計分子プローブ	菊地　和也	大阪大学・大学院工学研究科・教授	堀雄一郎 (00444563) 蓑島維文 (20600844)
A03 公	16H00770 超分子質量分析による蛋白質複合体の離合集散過程の解明	内山　進	大阪大学・大学院工学研究科・准教授	石井健太郎 (30748380) 野田勝紀 (大阪大学・大学院工学研究科・特任研究員)
A03 公	16H00772 アミロイド核の出現に先立つタンパク質初期集合および秩序化プロセスの解明	茶谷　絵理	神戸大学・大学院理学研究科・准教授	山本直樹 (90580671)
A03 公	16H00784 生物時計再構成系の動的秩序探究	寺内　一姫	立命館大学･生命科学部･教授	

A03 公	16H00786 無エンベロープウイルスの動的構造秩序形成の解析	村田　和義	生理学研究所・脳機能計測・支援センター・准教授	片山和彦 (60342903)
A03 公	16H00788 細胞膜受容体の動的会合体形成と分子認識反応	佐甲　靖志	国立研究開発法人理化学研究所・佐甲細胞情報研究室・主任研究員	
A03 公	16H00790 アミロイド線維の動的秩序形成過程の全貌の理論的解明	奥村　久士	自然科学研究機構・計算科学研究センター・准教授	伊藤暁 (90595381) 森義治 (90646928) 西澤宏晃 (日本学術振興会特別研究員)

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交付決定額（配分額）

	直接経費	間接経費	合計
平成 25 年度	243,400,000	73,020,000	316,420,000
平成 26 年度	259,100,000	77,730,000	336,830,000
平成 27 年度	237,000,000	71,100,000	308,100,000
平成 28 年度	224,600,000	67,380,000	291,980,000
平成 29 年度	220,700,000	66,210,000	286,910,000
平成 30 年度	3,000,000	900,000	3,900,000
総計	1,187,800,000	356,340,000	1,544,140,000

研究発表

(1) 雑誌論文（査読あり。共同研究の場合、重複あり。）

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A02：動的秩序の創生

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A03：動的秩序の展開

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A01：動的秩序の探査

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A02：動的秩序の創生

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【松浦友亮】

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12. Tomoaki Matsuura, “The time development of the protein synthesis involves a collapse and regrowth of the reaction network” QBic Symposium 2015, High-dimensional data for the design principles of life (RIKEN Quantitative Biology Center, 2016.8.24-26, Osaka
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4. Hiroyuki Miyake, Dynamic Structural Switching in Asymmetric Coordination Chemistry", Invited Seminar at Department of Chemistry, Gyeongsang National University, 2016.12.1, Jinju, Korea (Invited talk)
5. 三宅弘之, Dynamic Supramolecular Architecture via Asymmetric Coordination Chemistry, 錯体化学会第 66 回討論会シンポジウム,「Inorganic Molecular/Supramolecular Systems for Future Development of Photofunctional Materials」, 2016.9.10, 福岡 (Invited talk)
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A03：動的秩序の展開

【稲垣直之】

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9. 内山進「医薬品の熱測定」,2015 年 8 月 25～26 日,第 75 回熱測定講習会,京都府立大学,2015.8.25-26, 京都
10. 内山進 「水素重水素交換質量分析法による蛋白質の高次構造解析」, 第 34 回日本糖質学会年会,東京大学, 2015.7.31, 東京

11. 内山進,「抗体医薬などのバイオ医薬品の物理化学的評価」, 日本薬学会第 135 会年会, 2015.3.27, 神戸（招待講演）
12. Susumu Uchiyama , “Biophysical studies on antibody aggregation” JAACT international symposium, 2014.11.12, Kitakyu-shu （Keynote lecture）
13. 内山進,「抗体の物理化学的特性と抗体の凝集・機能性との関係」, 第 87 回 日本生化学会大会, 2014.10.18, 京都（招待講演）
14. 内山進, In solution characterizations of protein-protein interactions by analytical ultracentrifugation and mass spectrometry 第 52 回日本生物物理学会年会, 2014.9.26, 札幌（招待講演）
15. Susumu Uchiyama, “Biophysical factors governing antibody aggregation”, Workshop on Protein Aggregation and Immunogenicity., 2014.7.24, Breckenridge, Colorado（招待講演）
16. 内山進, 蛋白質相互作用・超分子複合体の質量分析 第 14 回蛋白質科学会年会 ランチョンセミナー, 2014.6.26, 横浜（招待講演）
17. 内山進, Analytical ultracentrifugation for quantitative intermolecular interaction studies, 第 14 回蛋白質科学会年会 ワークショップ, 2014.6.26, 横浜（ワークショップ主催）

【老木成稔】

1. Shigetoshi Oiki, Ion Permeation and Gating of the KcsA Potassium Channel Reconstituted in the Manipulated Membrane, Ion Channel Modulation Symposium 2017, 2017.6.21, Cambridge, UK (Keynote lecture)
2. Sumikama, T. and Oiki, S.: A 3-D movie of ion permeation through ion channel at the atomic levelfilmed by computer simulation. 94th Annual Meeting of the Physiological Society of Japan, 2017.3.28-30, Hamamatsu
3. 老木成稔：“人工膜マニピュレーション”第 38 回生体膜と薬物の相互作用シンポジウム ミニシンポジウム 1「人工膜を用いた研究最前線」名古屋市立大学 田辺通りキャンパス 2016.11.17-18, Nagoya
4. 老木成稔：カスタムメード膜でのチャネル研究法 カスタムメード膜でのチャネル研究法 第 63 回中部生理学会 特別プログラム「研究実験方法論」 岡崎コンファレンスセンター 2016.11.4-5, Okazaki
5. 老木成稔 チャネル研究のための人工膜法 自然科学研究機構プロジェクト・生理学研究所概算要求プロジェクト終了シンポジウム「次ステージ機能生命科学の展望」,2016, 岡崎
6. 老木成稔, チャネル研究のための人工膜法. 3 プロジェクト合同 終了シンポジウム「次ステージ機能生命科学の展望」, 岡崎コンファレンスセンター,2016.3.10, 岡崎
7. Shigetoshi Oiki, “Channel Function Reconstitution and Reanimation”, The 45th NIPS International symposium, Co-sponsored by “The Journal of Physiology” “Cutting-edge approaches towards the functioning mechanisms”, 2014.11.26-28, Okazaki (Invited talk)
8. 老木成稔, 「チャネル膜蛋白質 KcsA の一分子構造-機能ダイナミクスと膜」 膜学会「膜解析の最前線～生体膜・膜タンパク質から模擬膜,ソフトマターまで～」,2014.5.13, 東京 （招待講演）
9. Shigetoshi Oiki, “Spatio-Temporal Interplay of the Single KcsA Potassium Channel in the Membrane” OIST International Workshop: Single Protein Dynamics in Cellulo: Spatio-Temporal, Structural and Quantitative Analyses, 2014.4.21-25, Okinawa.（招待講演）

【岡本裕幸】

1. Yuko Okamoto, Generalized-ensemble simulations of biological molecular assembly and artificial molecular assembly, The 6th International Symposium on Dynamical Ordering of Biological Systems for Creation of Integrated Functions, 2018.1.20-21, Hamamatsu, Japan (invited talk)
2. Yuko Okamoto, Classical and quantum molecular simulations in generalized ensemble, International Workshop on Molecular Simulations, 2017.11.17-20, Nanjing, China(invited talk)
3. Yuko Okamoto, Generalized-ensemble algorithms for materials and biomolecular simulations Molecular Simulation Studies in Material and Biological Sciences (MSSMBS2017), 2017.9.7-10, St. Petersburg, Russia (Keynote lecture)
4. Yuko Okamoto, Generalized-ensemble algorithms for advanced materials simulations IUMRS-ICAM 2017, The 15th International Conference on Advanced Materials, 2017.8-27-9.1, Kyoto, Japan (invited talk)
5. Yuko Okamoto, Energy landscape of biomolecular systems studied by generalized-ensemble simulations, Energy Landscapes 2017, 2017.8.13-17, Goa, India, August (invited talk)
6. Yuko Okamoto, Efficient sampling methods for classical and quantum simulations, TSRC Workshop on the Chemistry and Dynamics in Complex Environments (CHEM-DiCE), 2017.6.26-30, Telluride, Colorado, U.S.A.(invited talk)

7. Yuko Okamoto, Biomolecular simulations in generalized ensemble, Frontier Bioorganization Forum 2017: Dynamical Ordering and Integrated Functions of Biomolecular Systems, 2017.4.24-26, Taipei, Taiwan(invited talk)
8. Yuko Okamoto, Generalized-ensemble simulations of complex systems, 2016 NCTS March Workshop on Critical Phenomena and Complex Systems, 2016.3.28-29, Hsinchu, Taiwan (invited talk)
9. Yuko Okamoto, Protein dynamics studied by generalized-ensemble simulations, The 251st American Chemical Society National Meeting, Symposium under the Computers in Chemistry (COMP) Division "30 Years of Protein Dynamics in Silico", 2016.3.13-17, San Diego, California, U.S.A. (invited talk)
10. Yuko Okamoto, Enhanced sampling methods for exascale computational chemistry, The 2015 International Chemical Congress of Pacific Basin Societies (PACIFICHEM2015), Symposium under the Physical, Theoretical & Computational Session, "Challenges and Opportunities for Exascale Computational Chemistry", 2015.12.15-20, Honolulu, Hawaii, U.S.A. (invited talk)
11. Yuko Okamoto, Generalized-ensemble algorithms for enhanced configurational sampling, Algorithms in Structural Bioinformatics: Sampling in Biomacromolecular Systems (AlgoSB Winter School - 2015), 2015.11.29-12.4, Cargèse, Corsica, France (invited talk)
12. 岡本祐幸, 「拡張アンサンブル法による量子化学シミュレーション」,分子研研究会「理論計算分子科学ワークショップ」, 2015.10.22, 岡崎市,日本 (招待講演)
13. Yuko Okamoto, Generalized-ensemble simulations of classical and quantum molecular systems, The 6th Japan-Czech-Slovak International Symposium for Theoretical Chemistry, 2015.10.11-15, Smolenice, Slovakia (invited talk)
14. Yuko Okamoto, Generalized-ensemble simulations, Hands-on Workshop on Computational Biophysics at Okazaki, 2015.9.9-11, Okazaki, Japan (invited talk)
15. 岡本祐幸,「古典系および量子系の拡張アンサンブルシミュレーション」,スーパーコンピュータワークショップ, 2015.9.7-8, 岡崎市,日本(招待講演)
16. Yuko Okamoto, Generalized-ensemble simulations of complex systems, 2015 NCTS International Workshop on Critical Phenomena and Complex Systems, 2015.8.15-17, Hsinchu, Taiwan (invited talk)
17. Yuko Okamoto, Generalized-ensemble algorithms for calculations of ligand binding affinity, BIRS Workshop: Free-Energy Calculations. A Mathematical Perspective, 2015.7.19-24, Oaxaca, Mexico, (invited talk)
18. Yuko Okamoto, Generalized-ensemble algorithms for enhanced sampling and free energy calculations Summer Snowmass Biophysics Workshop, Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics, 2015.7.5-9, Snowmass, Colorado, U.S.A. (invited talk)
19. Yuko Okamoto, Efficient sampling methods for identifying transition states
TSRC Workshop on the Chemistry and Dynamics in Complex Environments (CHEM-DiCE), Telluride, 2015.6.23-26, Colorado, U.S.A. (invited talk)
20. Yuko Okamoto, Efficient sampling methods for complex systems, The 19th International Annual Symposium on Computational Science and Engineering (ANSCSE19), 2015.6.17-19, Ubon Ratchathani, Thailand (Keynote lecture)
21. 岡本祐幸, 「拡張アンサンブル法による生体分子シミュレーション」, バイオスーパーコンピューティング名古屋 2015,2015.1.22, 名古屋（招待講演）
22. Yuko Okamoto, Lecture 1: "An introduction to replica-exchange molecular dynamics simulation"
Lecture 2: "Generalized-ensemble algorithms", The 11th Thai Summer School of Computational Chemistry 2015 Workshop:Replica Exchange Molecular Dynamics Simulation, 2015.1.4-7, Nan, Thailand (invited talk)
23. Yuko Okamoto, "Protein folding and ligand binding simulations by generaized-ensemble algorithms" The 7th Korea-Japan Seminars on Biomolecular Sciences – Experiments and Simulations, 2014.11.26-28, Seoul, Korea (invited talk)
24. 岡本祐幸, 「分子シミュレーションにおける拡張アンサンブル法」, 第８回分子シミュレーションスクール－基礎から応用まで－, 2014.10.14-17, 岡崎（招待講演）
25. Yuko Okamoto, "Protein folding and unfolding simulations by generalized-ensemble algorithms" Dushanbe Symposium on Computational Materials and Biological Sciences (DSCMBS-2014), 2014.9.23-28, Dushanbe, Tajikistan (Keynote lecture)

26. Yuko Okamoto, "Drug design by generalized-ensemble simulations", The 6th Japan-Russia International Workshop on Molecular Simulation Studies in Material and Biological Sciences (MSSMBS-2014), 2014.9.21-22, Moscow, Russia (Keynote lecture)
27. Yuko Okamoto "Computer simulations of protein folding, ligand binding, and proton transfer" 2nd International Conference on Computational Science and Engineering (2nd ICCSE 2014), 2014.8.21-23, Ho Chi Minh City, Vietnam (invited talk)
28. Yuko Okamoto, "Enhanced configurational sampling methods for spin systems and biomolecular systems"XXVI IUPAP Conference on Computational Physics, CCP2014, 2014.8.11-14, Boston, Massachusetts, U.S.A. (Keynote lecture)
29. Yuko Okamoto, "Enhanced sampling techniques for spin and biological systems", The 10th AIMS Conference on Dynamical Systems, Differential Equations and Applications Special Session "Enhanced Sampling Techniques in Simulation of Complex Systems", 2014.7.7-11, Madrid, Spain (invited talk)
30. 岡本祐幸, 「生体分子集団の相互作用と自由エネルギー計算」, 第 14 回日本蛋白質科学会年会, 2014.6.25-27, 横浜（招待講演）
31. 岡本祐幸, 「拡張アンサンブル法による分子シミュレーション」, 第 3 回産学連携シンポジウム「HPC の利用と成果と人材」,2014.1.31, 名古屋（招待講演）
32. Yuko Okamoto, "Reweighting techniques for Monte Carlo and molecular dynamics simulations" The 13th KIAS Protein Folding Winter School, High 1 Resort, 2014.1.19-24, Korea (Invited talk)
33. Yuko Okamoto, "Generalized-ensemble simulations of biological molecular assembly and artificial molecular assembly" The 2nd International Symposium on Dynamical Ordering of Biological Systems for Creation of Integrated Functions, 2014.1.11-12, Kyoto, Japan (Invited talk)
34. Yuko Okamoto, "Computer modeling of complex systems by generalized-ensemble simulations" The 2013 Hong Kong Workshop in Computer Modeling of Complex Processes, 2013.12.17-20, Hong Kong (Invited talk)
35. 岡本祐幸,「拡張アンサンブル法による生体分子の高次構造と機能の解明」, 物性研スパコン共同利用・CMSI 合同研究会（第 4 回 CMSI 研究会）,2013.12.11-13, 柏（招待講演）
36. Yuko Okamoto, Generalized-ensemble algorithms for molecular simulations, The 3rd International Conference on Molecular Simulation (ICMS 2013), 2013.11.18-20, Kobe, Japan (Invited talk)
37. Yuko Okamoto, "Enhanced-sampling simulations of spin and biological systems", West-Lake International Workshop on Statistical Physics and Complex Systems, 2013.11.8-10, Hangzhou, China (Keynote lecture)
38. Yuko Okamoto, "Generalized-ensemble algorithms for first-principles electronic structure calculations", 16th Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-16), 2013.10.27-30, Beijing, China (Invited talk)
39. 岡本祐幸, 「生体分子集団および人工分子集団の相互作用と大規模構造転換」 新学術領域研究「動的秩序と機能」第 1 回公開シンポジウム,岡崎,2013.10.2（招待講演）
40. Yuko Okamoto, "Generalized-ensemble simulations of spin and biological systems", The 1st International Symposium on Computational Materials and Biological Sciences, 2013.9.10-12, Tokyo, Japan, (Invited talk)
41. Yuko Okamoto, "Simulational physics in generalized ensemble",VII Brazilian Meeting on Simulational Physics, 2013.8.6-10, Joao Pessoa, Brazil (Invited talk)
42. Yuko Okamoto, "Generalized-ensemble algorithms for free energy calculations", Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics, 2013.7.15-19, Snowmass, Colorado, U.S.A. (Invited talk)

【奥村久士】

1. 奥村久士, アミロイド線維の生体分子動力学シミュレーション, 企業研究会第 31 期 CAMM フォーラム 本例会, 2018.1.12, 東京（招待講演）
2. Hisashi Okumura, Molecular dynamics simulations for aggregation and disaggregation of amyloid-ß peptides, EMN Meeting on Computation and Theory 2017, 2017.11.6-10, Dubai, United Arab Emirates (Invited talk)
3. 奥村久士, 分子動力学シミュレーションによるアミロイド線維の形成過程と破壊過程, 近畿化学協会コンピュータ化学部会例会, 2017.10.27, 大阪（招待講演）
4. Hisashi Okumura, Simulational studies of Aß amyloid fibrils by equilibrium and nonequilibrium molecular dynamics method, 21st International Annual Symposium on Computational Science and

Engineering, 2017.8.3-4, Pathum Thani, Thailand （Invited talk）

5. Hisashi Okumura, “All-atom molecular dynamics simulations of Aβ amyloid fibrils”, Institute for Protein Research (IPR) Seminar, Osaka University, Suita, 2017.1.26-27, Osaka, Japan （Invited talk）
6. Hisashi Okumura, “Equilibrium and nonequilibrium molecular dynamics simulations of Aβ amyloid fibrils”, 10th International Conference on Computational Physics, Holiday Inn, Sands Cotai Central, 2017.1.16-20, Macau, China (Invited talk)
7. Hisashi Okumura, “Dynamical ordering of amyloid fibril studied by molecular dynamics simulations”, Thai-Japan Symposium in Chemistry, Chiang Mai University, 2016.11.14-16, Chiang Mai, Thailand (Invited talk)
8. Hisashi Okumura, “Molecular dynamics simulations to study dynamical ordering of amyloid fibril”, 2016 NCTS October Workshop on Critical Phenomena and Complex Systems, National Tsing Hua University, 2016.10.5, Hsinchu, Taiwan (Invited talk)
9. Hisashi Okumura, “Molecular dynamics simulations of amyloid fibrils”, 2016 NCTS March Workshop on Critical Phenomena and Complex Systems, National Tsing Hua University, 2016.3.28-29, Hsinchu, Taiwan, (Invited talk)
10. 奥村久士, 「分子動力学シミュレーションによるアミロイド線維の離合集散」, 日本化学会特別企画「どこまで明らかになったか？自己組織化のメカニズム：アミロイド形成から人工系」, 同志社大学京田辺キャンパス, 2016.3.24-27, 京都（招待講演）
11. Hisashi Okumura, “Pressure induced structural change of proteins by molecular dynamics simulations”, Eighth Japan-Korea Seminars on Biomolecular Sciences, Institute for Molecular Science, 2016.2.15-17, Okazaki, Japan (Invited talk)
12. 奥村久士, 「分子動力学シミュレーションで探るアミロイドβペプチドの凝集,離散」国立長寿医療研究センター, CAMD セミナー, 2016.2.18, 愛知
13. Hisashi Okumura, “Molecular dynamics simulations of proteins under high pressure”, Pure and Applied Chemistry International Conference 2016, Bangkok International Trade & Exhibition Centre, 2016.1.9-11, Bangkok, Thailand (Invited talk)
14. Hisashi Okumura, “Molecular dynamics simulations for oligomerization and disruption of amyloid-β fibril”, The International Chemical Congress of Pacific Basin Societies 2015 (Pacifichem 2015), Hawaii Convention Center, 2015.12.15-20, Honolulu, Hawaii, USA (Invited talk)
15. Hisashi Okumura, “Nonequilibrium molecular dynamics simulation of amyloid-fibril disassembly by supersonic cavitation”, International workshop on complex phenomena from molecule to society, University of Tokyo, 2015.11.24-25, Tokyo, Japan (Invited talk)
16. 奥村久士, 「各種統計アンサンブルの生成法」, 第 9 回分子シミュレーションスクール—基礎から応用まで, 分子科学研究所, 2015.10.13-16, 愛知
17. 奥村久士,「アミロイド線維の分子動力学シミュレーション」第 2 回新学術領域研究「動的秩序と機能」若手研究会, 西浦温泉ホテルたつき, 2015.10.5-7, 愛知,（招待講演）
18. S. G. Itoh, New molecular dynamics simulation methods to enhance conformational sampling for biomolecules, 東京大学物性研究所 理論セミナー,2015.5.8, 柏 (Invited talk)
19. Hisashi Okumura, Nonequilibrium and generalized-ensemble molecular dynamics simulations for amyloid fibril, 11th International Conference of Computational Methods in Sciences and Engineering, 2015.3.20, Athens, Greece (Invited talk)
20. 奥村久士, アミロイド線維の形成初期過程と破壊の分子動力学シミュレーション
スーパーコンピュータワークショップ 2015, 2015.1.29, 岡崎（招待講演）
21. Hisashi Okumura, All-atom molecular dynamics simulations for amyloid fibril assembly and disassembly, The 3rd International Symposium “Dynamical ordering of biomolecular systems for creation of integrated functions”, 2015.1.11, Shima (Invited talk)
22. Hisashi Okumura, Thermodynamics and free energy calculation, 11th Thai Summer School of Computational Chemistry “Replica exchange molecular dynamics simulation”, 2015.1.7, Nan (Thailand) (Invited talk)
23. Hisashi Okumura, Molecular dynamics simulation and temperature replica-exchange method
11th Thai Summer School of Computational Chemistry “Replica exchange molecular dynamics simulation”, 2015.1.6, Nan (Thailand) (Invited talk)
24. Hisashi Okumura, All-atom molecular dynamics simulations of amyloid-fibril disruption and peptide oligomerization Mini Symposium, 2014.12.17, Okazaki (Invited talk)

25. 奥村久士, 生体分子系,液体系における分子動力学シミュレーション手法の開発と応用
第 28 回分子シミュレーション討論会, 2014.11.13, 仙台（学術賞受賞講演）
26. 奥村久士, Molecular dynamics simulations of Aß amyloid fibrils, 岡崎統合バイオサイエンスセンターリトリート, 2014.11.5, 岡崎（招待講演）
27. 奥村久士, アミロイド線維の破壊と形成初期過程の分子動力学シミュレーション
第二回 CUTE シンポジウム, 2014.10.30, 津（招待講演）
28. 奥村久士, 各種統計アンサンブルの生成法, 第 8 回分子シミュレーションスクール—基礎から応用まで—, 2014.10.15, 岡崎（招待講演）
29. Hisashi Okumura, Molecular dynamics simulations for amyloid fibril disruption and dimerization of amyloid-β peptides 2nd International Conference on Computational Science and Engineering,), 2014.8.22 Ho Chi Minh City, Vietnam (Invited talk)
30. Hisashi Okumura, Generalized-ensemble molecular dynamics simulations, 2014 UST-Sokendai Joint Seminar on Computational Sciences, 2014.7.31, Daejeon (Korea) (Invited talk)
31. 奥村久士, キャビテーションによるアミロイド破壊の非平衡分子動力学シミュレーション
山手イブニングセミナー, 2014.6.6, 岡崎（招待講演）
32. Hisashi Okumura, Generalized-ensemble algorithms to determine free-energy landscape of proteins10th International Conference of Computational Methods in Sciences and Engineering, 2014.4.4, Athens, Greece (Invited talk)
33. S. G. Itoh and H. Okumura, Free-energy calculation by the replica-permutation method for biomolecules, 10th International Conference of Computational Methods in Sciences and Engineering, 2014.4.4, Athens, Greece (Invited talk)

【加藤晃一】

1. Takumi Yamacguchi, Design and creation of neoglycoconjugates for the application of biofunctional oligosaccharides, JAIST Japan-India Symposium on Materials Science 2018 2018.3.5, 能美(Invited talk)
2. 佐藤匡史, 加藤晃一, 糖タンパク質品質管理メカニズムの構造基盤解明, 第 46 回結晶成長国内会議（JCCG-46）2017.11.28, 浜松（Invited talk)
3. Koichi Kato, Structural aspects of glycosylation as potential drug target, The 19th Symposium on Advanced Concepts in New Drug Developmemt : 1st Ewha-NCU Joint Symposium, 2017.11.16, Seoul(Invited talk)
4. Koichi Kato, Isotope Labeling Approaches for Carbohydrates and Glycoproteins, 第 56 回 NMR 討論会, 2017.11.15, 八王子(Invited talk)
5. Koichi Kato, Dynamic ordering of biomolecular systems coupled with creation of integrated functions CU-IMS collaborative seminar, 2017.10.31, Bangkok (Invited talk)
6. Koichi Kato, Dynamic ordering of biomolecular systems coupled with creation of integrated functions The NANOTEC-IMS Joint Research Meeting, 2017.10.30, Pathum (Invited talk)
7. Koichi Kato, Maho Yagi-Utsumi, Saeko Yanaka, Tatsuya Suzuki, Hirokazu Yagi, Tadashi Satoh, and Takumi Yamaguchi, Structural mechanisms of carbohydrate functions, Taiwan-Japan Biomedical Symposium on Magnetic Resonance, 2017.10.15, Tainan (Invited talk)
8. Kensuke Kurihara, Constructive biology approach to artificial cells: Artificial cells based on vesicles from nonliving materials, 6th International Conference in Biology, Chemistry and Agronomy, 2017.9.27, Guadalajara, Mexico (Keynote lecture)
9. 加藤晃一, 抗体を源流とする生命分子構造学の展開, 静岡県立大学薬学部 第 264 回 月例薬学セミナー, 2017.9.22, 静岡
10. 矢木宏和, 谷中冴子, 與語理那, 鈴木達哉, 山口拓実, 杉山正明, 加藤晃一, 統合的な構造物学アプローチによるに糖タンパク質および糖鎖の構造ダイナミクスの解析, Integrative structural biology approaches for understanding conformational dynamics of oligosaccharides and glycoproteinsm 第 55 回 日本生物物理学会年会, 2017.9.20, 熊本
11. 加藤晃一, 糖鎖の生命分子科学の探究, 第11回 分子科学討論会, 2017.9.17, 仙台
12. Saeko Yanaka, Stable isotope labeling for NMR observation of antibody glycoproteins in serum environments, Seminar at Max Planck Institute for Biophysical Chemistry, 2017.9.14, Göttingen (Invited talk)
13. Koichi Kato, Structural views of fate determination of glycoproteins in cells, Seminar at Max Planck Institute for Biophysical Chemistry, 2017.9.14, Göttingen (Invited talk)

14. Saeko Yanaka, Integrative approach for exploration and creation of dynamical ordering of biomolecular systems, 14th HORIZONs in Molecular Biology, 2017.9.11-14, Göttingen (Invited talk)
15. 矢木宏和, 糖タンパク質糖鎖の構造解析法の開発と糖鎖機能解析への応用, 第 2 回 G-CHAIN セミナー, 2017.9.8, 岐阜
16. 佐藤匡史, 鈴木達哉, Gengwei Yan, 谷中冴子, 矢木宏和, 山口拓実, 加藤晃一, レクチンによる動的な糖鎖の認識機構, 第 4 回レクチン研究会, 2017.9.4, 東京（招待講演）
17. Hirokazu Yagi, The characterization of the laminin-binding glycans on alpha-dystroglycan catalyzed by several causative gene products of dystroglycanopathy, The 1st International Conference on the Glycobiology of Nervous System, 2017.9.2, Seoul (Invited talk)
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A01：動的秩序の探査

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研究成果による産業財産権の出願・取得状況

A01：動的秩序の探査

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A02：動的秩序の創生

【平岡秀一】

1. 「ヘキサフェニルベンゼン骨格の位置選択的交互型修飾方法」、発明者：平岡秀一、小島達央、権利者：国立大学法人東京大学, 番号：特願 2014-45233, 出願日： 2014 年 3 月 7 日, 国内外の別：国内

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A03：動的秩序の展開

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2. 「タンパク質を蛍光標識する方法」, 権利者：国立大学法人大阪大学, 発明者：水上進, 渡辺修二, 秋元悠里, 菊地和也, 特許番号：特許第 5686385 号, 登録日：2015 年 1 月 30 日

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【重田育照】

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研究成果

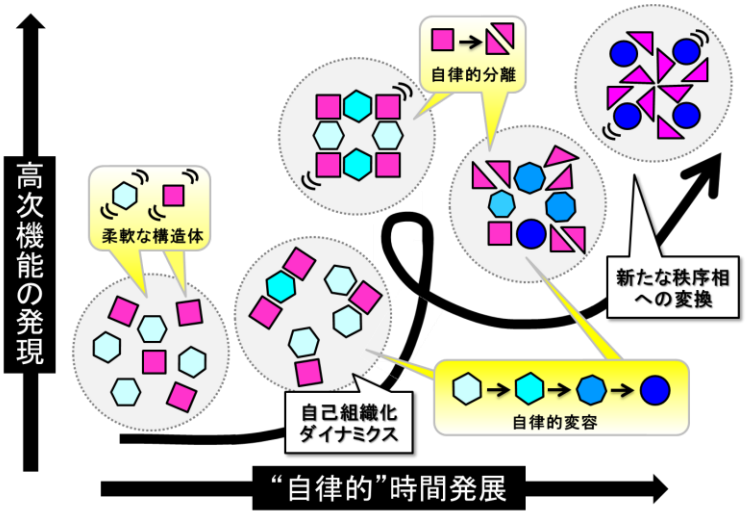
研究領域の目的及び概要

研究の学術的背景　着想に至った経緯

生命現象の特徴は、システムを構成する複数の分子素子がダイナミックな集合離散を通じて秩序構造を形成し、それが自律的に時間発展していくことにある。生命体を構成する個々の分子素子は、それぞれが複雑な 3 次元構造と独特の柔構造を有している。すなわち、内的複雑性を秘めた分子素子が多数集積して協奏的に高次秩序系を体現していることが生命体の特質であり、その形成原理を解明することが生命現象の本質的理解につながるはずである。

生命体の秩序は、歴史的には Schrödinger の思索において negentropy という概念で表出され、Prigogine らによって散逸構造の一形態として取り扱われてきた。当然のことながら、こうした概念は今日明らかとなっている生命分子の多様性や複雑性を念頭に置くものではない。前世紀末期に勃興したゲノムサイエンスの潮流は、‘omics’と称されるアプローチによる生命情報の網羅的集積を推進してきた。実際、今世紀に入りタンパク質の立体構造データは爆発的な勢いで蓄積されており、生命素子間の相互作用ネットワークを基盤とするシステム生物学も急速に発展してきた。しかしながら、それら生命素子がダイナミックな相互作用を通じて時空間的秩序を形成し機能発現する仕組みを分子科学に立脚して理解することを目指した取り組みは驚くほど少ない状況であった。

一方、1990 年代より分子の自己組織化を主題とする超分子化学の研究領域が目覚ましい発展を遂げてきた。これは、巧妙にデザインされた低分子が自発的に集積する性質を利用して一定の空間的秩序を有するナノ構造体の構築を目指すものである。こうした研究は、これまでかならずしも生命システムとの積極的な関連付けを企図して行われてきたわけではないが、自己集積を通じて個々の要素が持ちえない高次機能を創発するという点において生命システムと通底する。但し、いうまでもなく、生命分子の自己組織化は、非生体系の場合と比して遥かに複雑である。それは、上述のように個々の要素分子が複雑な動的高次構造を有するということもさることながら、多種類の分子が弱い相互作用を通じて自己集積し、非対称性と可塑性を有する動的秩序構造を形成するということによる。こうした性質は、生命機能の発現と密接に関係している。さらに、生命超分子集合体は、外部環境の変動や超分子集合体間の自律的なコミュニケーションを通じて時空間的発展を遂げる。そのスケールは空間的にはサブミクロン、時間的には日（day）のオーダーに及ぶこともある。このような生命分子集団の振る舞いについての統合的理解に向けた分子科学的取り組みはポストゲノムがうたわれて久しいにも関わらず実現しておらず、とりわけ生体分子研究者と非生体系研究者との体系的な知的連携はなされていなかった。



以上の学術的背景のもとに、生命分子が動的な秩序を形成して高次機能を発現する仕組みを分子科学の観点から解き明かし、それを通じた生命現象の本質的理解を目指して本研究を提案した。さらに、先端生命分子科学と超分子化学のアプローチを融合することによって、生命分子システムの特質を具現化した動的秩序系を人工構築することを目指した。

領域申請の理由　本領域の発展による学術水準の向上

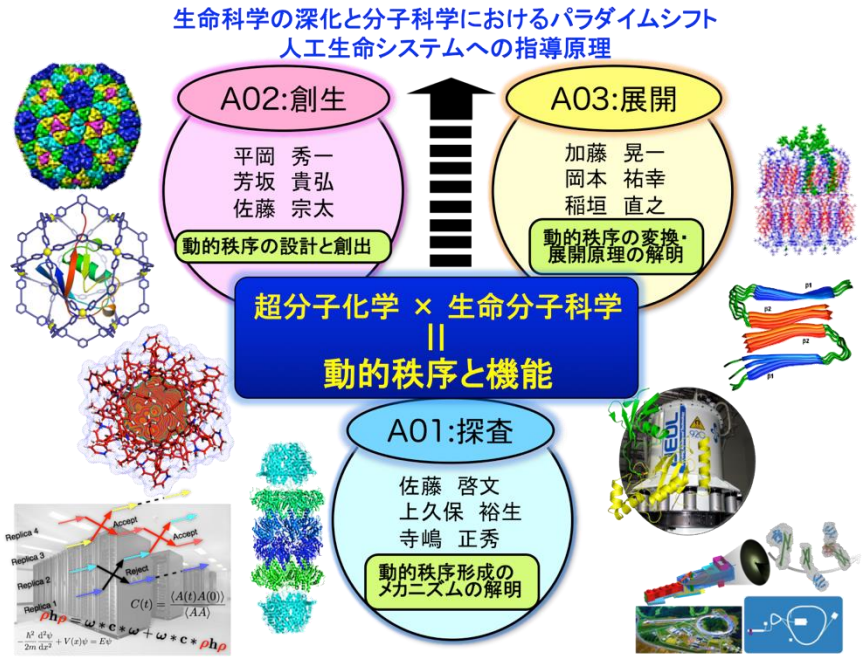
以上の目的を実現するためには、生命超分子系という巨大な森の相の変動を見つめつつ、それを構成する木々の個々の枝葉の振る舞いを捉え、両者を相関づけるアプローチが必要である。そのために、生命分子科学を基軸に、生物物理学、理論・計算科学、合成化学、構造・システム生物学、さらには医学・薬学・工学・環境科学等への応用を見据えた研究体制を構築する。現在、国際的にも生命分子の構造・機能データベースが充実し、我が国においても計算科学と実験科学を支援する大型施設が拡充している。こうした時機を鑑みても、多様なバックグラウンドの研究者が明確な問題意識を共有して叡智を結集し、生命分子の動的秩序形成の理解に向けた分野横断的な研究体制を組むことの意義は大きい。

本研究領域は、生命分子科学と自己組織化の化学の融合により、生命現象の諸相にみられる分子の秩序形成の原理を統合的に理解するとともに、その人工構築を目指すものである。その成果は、創薬をはじめとする応用研究の進展に資するばかりでなく、生命科学一般の深化と分子科学におけるパラダイムシフトをもたらし、人工的な生命システムを創生するための指導原理を導き出すことが期待される。したがって、本領域が成功裡に進展することにより、他の研究領域の発展にも極めて大きな波及効果がもたらされる。

研究の概要

本領域では、**分子が自律的に集合するプロセスについて精密に探査することを可能とする実験と理論の融合研究を実施した**（研究項目 A01「動的秩序の探査」）。また、**生命分子科学と超分子化学のアプローチを統合することを通じて、生命分子システムの特質を具現化した動的秩序系を人工構築した**（研究項目 A02「動的秩序の創生」）。さらに、**生命分子の自己組織化系の設計原理を明らかにするとともに、外的摂動に対するシステムの不安定性とロバストネスを解明することを通じて、高次機能発現に至る時空間的展開の原理を理解することに取り組んだ**（研究項目 A03「動的秩序の展開」）。

上記各項目において、各メンバーが独自の生命分子システムを対象に研究を進めるとともに、いくつかの特定の対象をターゲットとして、項目横断的な研究連携も推進した。その主な対象としては、細胞内のタンパク質の運命（立体構造形成・輸送・分解）にかかわる超分子マシナリー、細胞表層における糖鎖・脂質・タンパク質からなる超分子系、アルツハイマー病をはじめとする神経変性疾患にかかわるタンパク質の会合体形成、概日リズムを司る時計タンパク質複合体などを取り扱った。また、非生体分子を基盤に構築された人工的な分子集合システムについても、生体分子系と同様に精密な実験計測と理論的アプローチを展開してそのダイナミクスを明らかにし、時空間的非対称性と散逸性を有する動的秩序形成に向けての分子設計上の指針を得た。



本領域の目的を達成するために、生命分子システムにおける動的秩序の探査（A01）・創生（A02）・展開（A03）の 3 つの研究項目を研究の柱として設定し、それぞれの項目について化学・物理学・生物学の分野横断的な連携研究と、新規方法論の開発を含めた実験と理論の融合研究を実施し、下記の通り順調に成果を上げた。

A01 生命システムが現有する動的秩序構造を捉えるための計測技術の開発・高度化を通じて、その形成過程の精密観測を達成し、理論と実験の両面から動的秩序形成のメカニズムを解き明かした。

A02 実験・理論の両面から生命システムの動的秩序を再構築するとともに、自己集積能を有する非生体系分子に生命分子の特質を賦与することにより、人工的な動的秩序形成系を創成した。

A03 生命分子の自己組織化系の設計指針を明らかにし、外的摂動に対するシステムの不安定性とロバストネスを解明することを通じて離合集散を経て高次機能発現に至る時空間的展開の仕組みを理解した。

このように、**研究領域として設定した目的は十分に達成されたが、特筆すべきことは、各研究項目の枠組みを超えた共同研究が活発に行われたことで、期待以上に多くの成果を収めたことである。**

1. 人工系と生体分子系に底通する自己集合の普遍性の解明

分子自己集合も化学反応の 1 つであるが、多くの中間体が生成する上に、これらを実験的に観測することが難しい。そのため、本研究領域が発足した当時、分子自己集合過程に関する分子論的解明は全くと言って良いほど進んでいなかった。分野融合的な研究を推進することにより、人工系および生命分子系の自己集合機構を分子論的に解明するためのアプローチ法を確立し、両者に通底する自己集合の普遍性を明らかにすることができた。この成果は、人工的な生命システムを設計・創生するための指導原理を確立する基盤を築くものである。

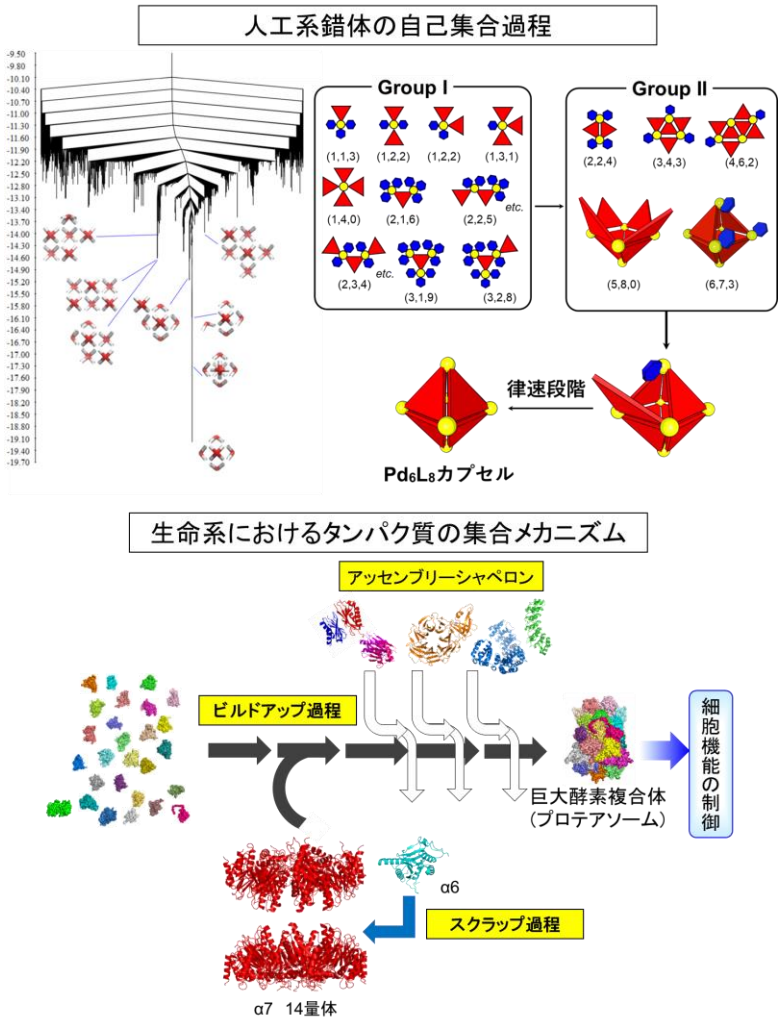


図 1. 人工系および生命系における一義自己集合体の形成機構の解明. (上)理論的なアプローチと実験的アプローチを合わせることで，自己集合過程で生成する観測不可能な中間種の同定に成功. (下)プロテアソームの自己集合過程におけるアッセンブリーシャペロンの役割を解明するとともに，スクラップ・アンド・ビルド過程の存在を見出した.

平岡（A02 計画）は、分子自己集合過程で生成する中間種を検出できないという問題を解決し、自己集合過程を解明する解析法（QASAP: Quantitative Analysis of Self-Assembly Process）を開発した。これは、自己集合の原系と生成系の全成分を定量することで、全中間種の平均組成を間接的にあぶり出す手法であり、原理的に様々な分子自己集合に応用可能である。QASAP を自己集合性錯体に適用し、14 種類に及ぶ自己集合体の形成機構を解明することで、分子自己集合がエネルギーランドスケープ上を様々な経路を経て進行することを明らかにした。そして、佐藤(啓)（A01 計画）はマスター方程式を使った自己集合過程に迫る新しい理論手法を開発し、これらの自己集合性錯体のより詳細な形成機構

を理論的に解明した。このように、実験と理論の協働により、人工分子の自己集合過程がタンパク質のフォールディングと相同性をもつことを明らかにした（図 1）。さらに、佐藤(啓)は量子化学計算や REST（replica exchange with solute tempering）法を使って、平岡が開発した箱型六量体「ナノキューブ」の自己集合過程を理論的に解明することにも成功した。ナノキューブは疎水効果やファンデルワールス力などの生命系で頻繁に利用されている弱い因子により集合化しているため、この自己集合体の形成過程の理解は、生命系の自己集合過程の理解に繋がるだけなく、生命分子の特性を兼ね備えた人工分子のデザイン指針の確立にも欠かせない。

一方、加藤（A03 計画）は、複雑な生命系におけるタンパク質分子の自己集合過程として、多数のサブユニットから構成されるタンパク質分解装置プロテアソーム複合体の動的秩序形成機構の解明に向けて、各パーツ分子の動的秩序形成におけるミクロ-マクロ相関を探査した。プロテアソームの分子集合に一過的に関わる一連のアッセンブリーシャペロンがサブユニットの適切な配置を定める“チェックポイント”や“分子マッチメーカー”として機能していることを解明した。さらに、プロテアソームの 4 次構造形成にスクラップ・アンド・ビルドのプロセスが織り込まれることにより、精密な分子集合が可能になっていることを明らかにした（図 1）。

これに呼応するかのように、平岡は、人工分子の自己集合過程で一過的に生成する中間種の中には、最終構造の 50 倍以上も大きい種が形成することや、非対称化された準安定種が存在することを突き止めた。さらに、構成成分では無い分子の介在が自己集合に必須である系も見出し、生命系におけるシャペロンに近い機構が人工系にも存在することを明らかにした。これにより、人工系と生体分子系における自己集合の普遍性がより明確に浮き彫りとなった。

2. 分子集合のエネルギーランドスケープにおける速度論支配と熱力学支配の制御

分子自己集合には上記のような一義自己集合体の他に、線維やシートなど、ある次元について無限に広がる自己集合体もある。これらは、動的秩序形成の普遍性を論ずるのに格好の題材であり、その形成機構についても人工系および生命系の実験と理論研究者が共同で問題に取り組むことで重要な知見が得られた（図 2）。杉安（A02 公募）は、ポルフィリン環に置換基を導入した分子が、はじめに微粒子を速度論的に形成し、これが単量体への解離平衡を経て熱力学的に安定な線維構造へ変換することを発見し、さらに導入する置換基をわずかに変化させるだけで、シート構造を生成することに成功した。これらの成果は、分子集合のエネルギーランドスケープにおける速度論支配と熱力学支配を制御することで超分子形成の時間発展のプログラミングが可能であることを示した。

生命系において、茶谷（A03 公募）はタンパク質の線維状集合体の形成過程で線維前駆中間体が一過的に生成することを見出し、この中間体の同定にも成功した。さらに、線維前駆中間体に先駆けて生成する粒子状集合体の検出にも成功し、特定の中間体についてのみ超音波照射により線維形成を引き起こす活性種へ変換できることを明らかにした（図 2）。また、奥村（A03 公募）はハミルトニアン置換分子動力学シ

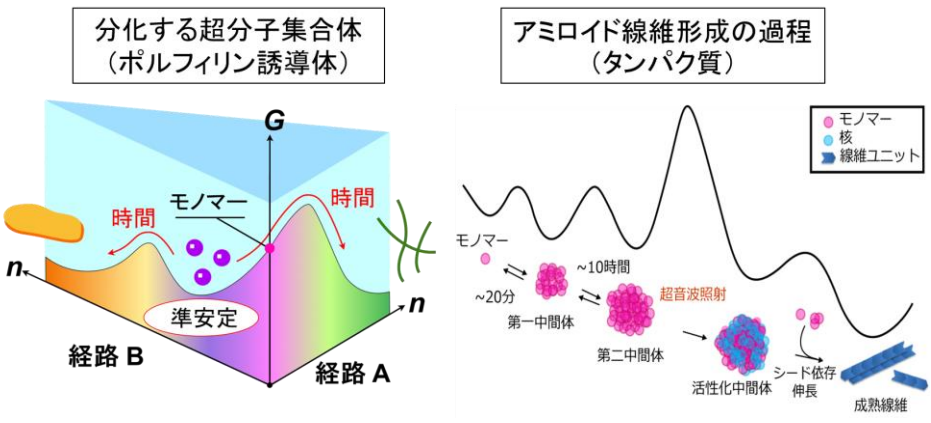


図 2. 人工系および生命系における線維やシートの自己集合過程の解明.
「人工分子の自己集合におけるエネルギーランドスケープのコントロール(左)」と「タンパク質の集合化による線維状自己集合体の形成機構(右)」には高い類似性があり，人工系と生体分子系に普遍な自己集合の原理が見出された.

ミュレーションによって、タンパク質の線維形成のシミュレーションに成功し、単量体が接近することでヘアピン構造が増加し、分子間のシート構造が増えることを見出した。さらに、この 2 量体に単量体が結合することで三量体、四量体と成長し、核へ単量体が結合することで集合化が進む機構で線維形成が起こることを突き止めた。このように、これまで異なるものとして認識されていた現象が、本領域の活動を通じて体系的に理解できるようになり、その根底に共通する機構に基づいて分子集合をプログラムすることが可能となった。

3. 非平衡系における分子の離合集散による秩序形成の理解

生命系の特徴は、一度形成された秩序構造が安定に維持されるだけでなく、集合・解離を繰り返すことで、動的に秩序を生み出していることである。本研究領域では、このような系についてもミクロとマクロのダイナミクスをつなぐ理解を促した　(図 3)。

時計タンパク質は 24 時間という長い周期で離合集散を繰り返し、概日リズムを司っている。秋山(修)（A01 公募）はシアノバクテリアの生物時計を構成する Kai C タンパク質に 24 時間の周期を司る機構が存在することを突き止め、長い周期を刻む分子機構が、立体的な要因とペプチド鎖の異性化という 2 つの因子が ATP の加水分解を極端に遅らせていることに起因することを明らかにした。稲垣（A03 計画）は神経細胞における軸索の形成機構の解明に取り組み、アクチン線維が神経細胞の伸長方向へ重合し、後方で脱重合するアクチン波が起こる際に、細胞接着タンパク質を介して細胞外基質に連結されるという従来のモデルを覆す新しい機構であることを明らかにした。さらに、神経軸索が誘引分子を検知して軸索を伸長させるための力を生み出す仕組みも解明した。このように、生命系における離合集散の分子論的理解が飛躍的に進んだが、併せて、人工系においても周期を刻み律動する分子を開発することに成功した。鈴木（A02 公募）は Belousov-Zhabotinsky（BZ）反応を温度応答性の高分子と複合化することで、周期的に自律駆動するゲル微粒子を開発した。また、その作用機構を解明するとともに、高田（A01 公募）との共同研究を通じて、ゲル微粒子の架橋点にロタキサン構造を導入することで、pH と温度といった複数の刺激に対してそれぞれ応答できるようになり、生命系に迫る動秩序系を構築することにも成功した。

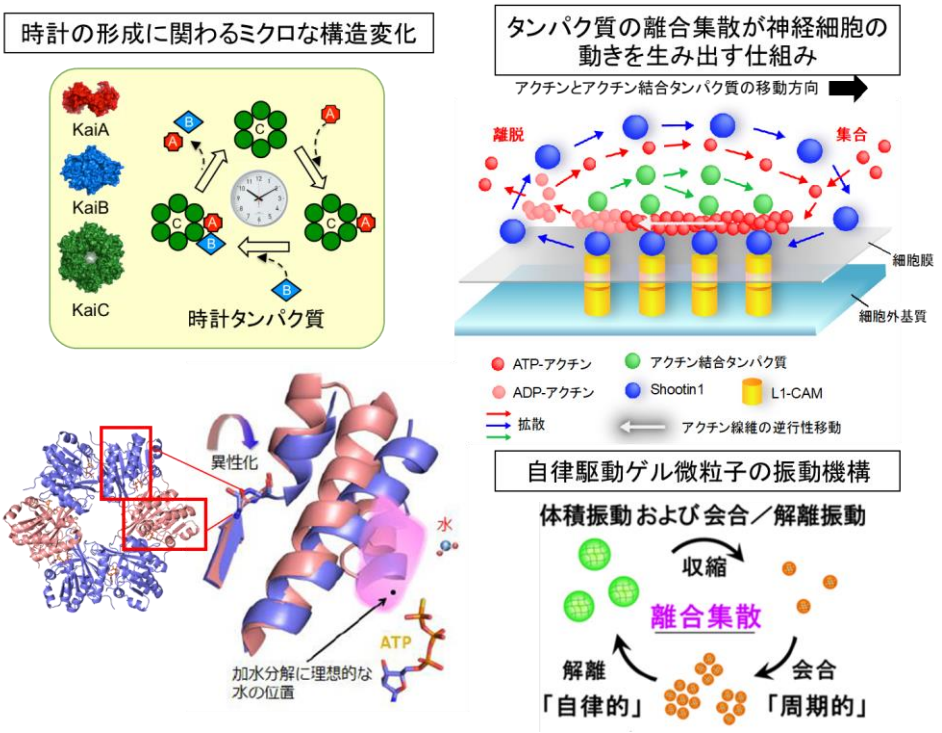


図 3. 離合集散を繰り返す動的な秩序形成の機構の解明．時計タンパク質のうち，KaiC が 24 時間のリズムを司り，この長い周期をコントロールする分子機構が明らかになった．また，神経軸索の形成におけるアクチン波の新規機構を解明した．さらに，温度と pH という 2 種類の外的因子に独立して応答する自立駆動ゲル微粒子の創出が実現した．いずれも離合集散により同調的に周期的律動をする分子システムの理解につながる成果である．

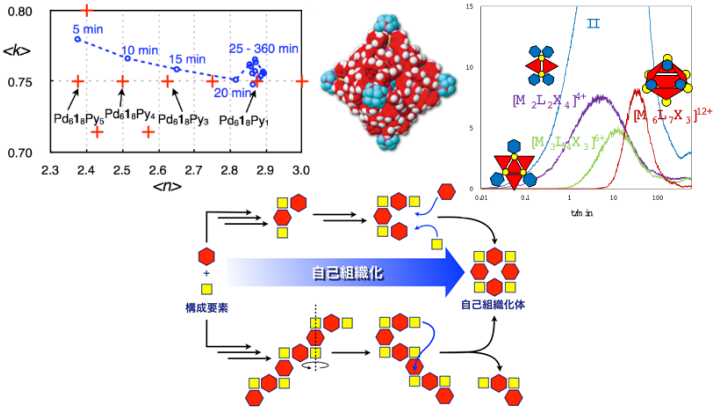
本領域は、人工系と生命分子系の動的秩序形成に本質的な相同性を見出し、両者に通底する自己集合の原理を浮き彫りにすることができた。さらに、非平衡系における生体分子の離合集散過程について、実験と理論の両面から詳細に解き明かした。それらの特質を備えた人工分子の創生や、同調的に周期的律動をする人工高分子ゲルや生体分子と人工超分子のハイブリッド化による高次機能の創出にも成果を収めた。
このように、提案当初に掲げた目標を十二分に達成することができた。

主な研究成果

研究項目 A01「動的秩序の探査」

動的秩序形成を探査する分子理論のアプローチ法を開拓し、超分子の自己組織化メカニズムを解明

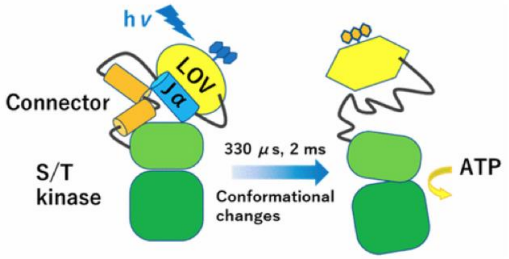
主な発表論文：*Phys. Chem. Chem. Phys.* 2018【A01 佐藤(啓)、A02 平岡の共同】、*Phys. Chem. Chem. Phys.* 2018【A01 立川、A01 重田、A02 平岡の共同】、*Chem. Eur. J.* 2017【A01 立川、A02 平岡の共同】



理論を担当する佐藤(啓)（A01 計画）は、平岡（A02 計画）と協力しながら、自己集合過程の物理化学的原理の解明に取り組み、秩序形成過程をマスター方程式や量子化学計算によって追跡する方法を提案した。これにより、自己集合過程の実験的観測を実現した平岡の成果をサポートするだけでなく、中間体の生成・分解の経時変化や、自己集合律速段階をコントロールする因子を解析し、秩序形成のメカニズムを明らかにした。また、立川や重田（ともに A01 公募）は、量子化学計算や MD 法を駆使し、溶媒効果が会合体の安定性や動態に与える影響や、分子自己集合過程における速度定数や活性化エネルギーを求めることに成功した。

タンパク質の過渡的相互作用を捉え、マルチドメインタンパク質の作動原理を解明

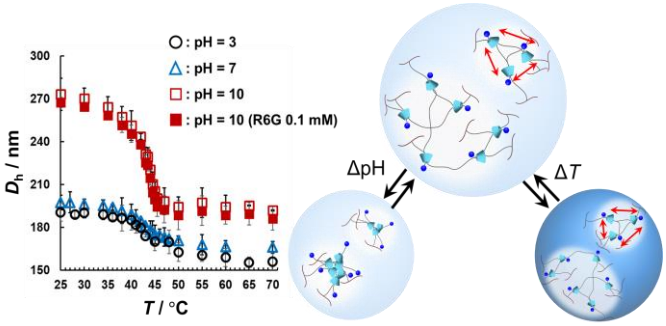
主な発表論文：*J. Phys. Chem. B* 2017【A01 寺嶋】、*Sci. Rep.* 2017【A01 上久保、A01 内橋、A03 加藤、A03 村田の共同】、*J. Am. Chem. Soc.* 2016【A01 寺嶋、A02 神谷の共同】



タンパク質が機能を発揮する際には、内部のミクロ構造変化のみならず、様々な機能をもったモジュール構造のマクロな時空間的変化が重要な鍵となる。寺嶋（A01 計画）は、独自に開発した過渡回折格子法を武器に秩序構造ダイナミクスを追跡し、巨大なマルチドメイン構造をもつ光センサータンパク質が局所構造を維持しつつドメイン間の空間配置を変化させる様子の時間分解測定に成功した。さらに本手法を神谷（A02 公募）が開発した光応答性人工核酸システムと組合わせ、DNA2 重差構造の解離過程の詳細を解明することにも成功した。上久保（A01 計画）は、多成分系の溶液散乱データの系統的収集を実現する微小量自動サンプリングシステムを開発した。領域内の 4 グループ（上久保、内橋（A01 公募）、加藤（A03 計画）、村田（A03 公募））が連携することで、溶液散乱計測や高速 AFM 観察による動的構造解析と、電子顕微鏡、結晶構造解析の静的観察結果を統合し、細胞内秩序維持に関わる小胞体フォールディングセンサー酵素の、柔軟なモジュール構造を巧みに用いた作動機序を明らかにした。

“お互いに干渉し合わない”多刺激応答性ゲル微粒子の実現

主な発表論文：*Angew. Chem. Int. Ed.* 2017【A01 高田、A02 鈴木の共同】、

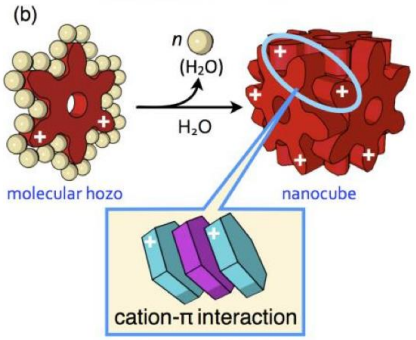


生命活動の維持には、複数の刺激に適切に応答し、構造や機能の変化を行うことが不可欠である。こうした動的秩序システムの人工系での実現を目指し、高田（A01 公募）は鈴木（A02 公募）と協力して多刺激応答性を有するソフトマテリアルを創出した。人工系での分子設計においては、1 つの刺激に対応すると、他の刺激応答性が著しく消失してしまうという問題が生じやすい。そこでロタキサン構造に由来する環動性をゲル微粒子に導入することで問題を克服し、温度と pH の変化に対し相互不干渉に応答する分子システムを実現した。

研究項目 A02「動的秩序の創生」

弱い相互作用を積み上げて高次構造体を創生

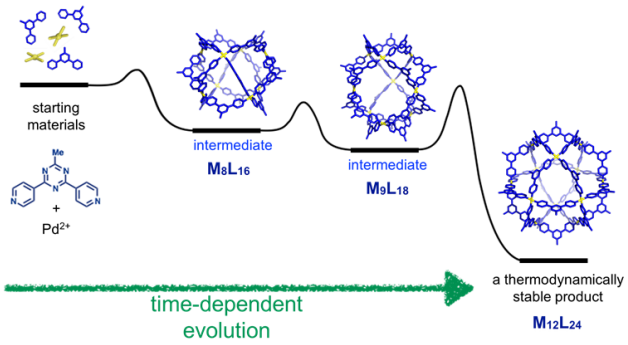
主な発表論文： *Commun. Chem.* 2018【A01 立川、A02 平岡、A03 内山の共同】、*Chem. Comm.* 2017【A01 岩田、A01 松森、A02 大谷の共同】、*Nature* 2016【A02 佐藤(宗)】



生命分子システムの動的秩序化においては、疎水効果やファンデルワールス力などが無数に集積することで強大な束縛力を産み出す。人工系においてもこうした弱い相互作用を制御することで高次構造体を創出するとともに、物理化学計測を通して秩序形成のメカニズム理解の深化を図った。平岡（A02 計画）は、立川（A01 公募）とともに分子同士の噛み合わせを評価する手法を確立した。ここから得られた知見をもとに精密設計した歯車状分子の自己組織化を通して、超好熱菌由来タンパク質の熱耐性をも上回る安定性をもった超分子を開発することに成功した。佐藤(宗)（A02 計画）は配位結合によって 140 を超える構成成分からなる人工分子を創出し、X 線結晶構造解析を通して、構成成分数の増加に伴い従来の安定な幾何学的制約を打ち破る秩序が新たに創出されることを発見した。また大谷（A02 公募）は、金属錯体を含む人工脂質からなるリポソームを設計するとともに、岩田や松森（ともに A01 公募）との連携による脂質ダイナミクス解析を通して、表面は硬く内部は柔らかいという膜構造の不均一性を明らかにした。

超分子集合体形成の時間展開の発見と制御

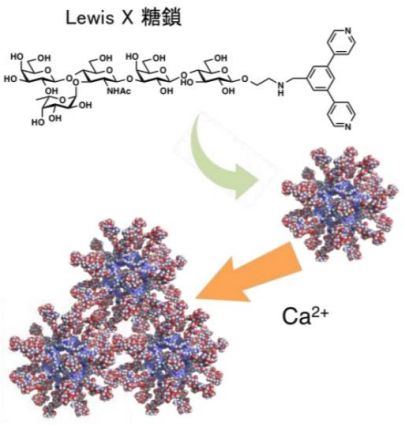
主な発表論文：*Nature Chem.* 2017【A02 杉安】、*Angew. Chem. Int. Ed.* 2015【A02 佐藤(宗)】



佐藤(宗)（A02 計画）は、時間展開する動的な秩序化システムの過程を、中間体構造の実験的な構造決定も含めて解明し、36 成分からなる金属錯体分子の自己組織化の過程が、実は、幾何学的に制約されることで簡素化されて、たった 2 種類の準安定な中間体構造を経て、単一の生成物に落ち着く、明瞭なシステムであることを明らかにした。また杉安（A02 公募）は、分子デザインを通して熱力学的な準安定状態を利用して秩序化を制御することに成功し、1 つの初期状態から全く異なる 2 つの終状態へ分化する超分子の創生や、超分子集合体形成の時間発展プログラミングを実現した。

サイボーグ超分子を創生して糖鎖クラスターの相互作用の観測に成功

主な発表論文：*Chem. Asian J.* 2017【A02 佐藤(宗)、A03 加藤の共同】、*Angew. Chem. Int. Ed.* 2015【A02 佐藤(宗)、A03 加藤の共同】



佐藤(宗)（A02 計画）と加藤（A03 計画）は、生体分子と人工超分子のハイブリッドによるサイボーグ超分子を創生し、アルツハイマー病の発症にかかわるアミロイド β タンパク質と糖鎖クラスターとの相互作用解析に応用した。さらに、機能性糖鎖を組み込んだ人工分子クラスターのデザインを発展させ、外部環境に応答して高次の離合集散を行う性質を賦与した超分子複合体を創生した。外部環境に応じた離合集散の過程においては糖鎖—糖鎖間の分子認識が重要な役割を担うことを明らかとした。

人工細胞システムの創出と応用

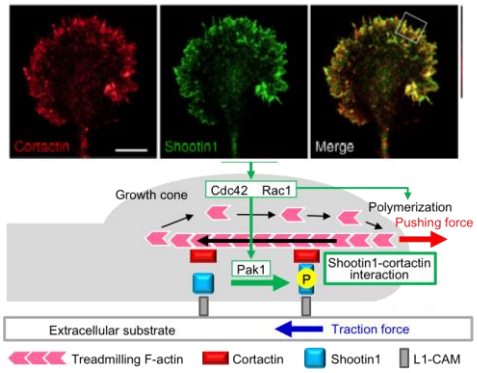
主な発表論文：*Proc. Natl. Acad. Sci. USA* 2017【A02 松浦】、*Chem. Commun.* 2016【A03 栗原】、*ChemBioChem* 2015【A02 芳坂、A02 松浦の共同】

生体分子や人工分子を組み合わせて構成した人工細胞の創出と応用も進んだ。芳坂（A02 計画）と松浦（A02 公募）は、人工細胞システムを用いた進化分子工学手法によりタンパク質を改良・進化させ、非天然アミノ酸を導入するための高機能型 tRNA 合成酵素を作り出すことに成功した。さらに松浦は、細胞モデル中での 241 成分の濃度変化を計算し、タンパク質合成反応をシミュレーションするプログラムを開発し web 上に公開した。また栗原（A03 計画分担）は人工細胞モデルの化学的進化を進め、生命の必須要素である代謝のための触媒が内在し、自己生産するベシクルを合成した。

研究項目 A03「動的秩序の展開」

力と分子の滑りを利用した神経ネットワーク形成の新しい仕組みを解明

主な発表論文：*Proc. Natl. Acad. Sci. USA,* 2018【A03 稲垣】、*Cell Reports* 2015【A03 稲垣、A03 水野の共同】



神経細胞は、脳内の分子の濃度勾配に導かれて軸索を伸ばし、適切な神経細胞と結合することで脳の活動に必要な神経ネットワークを作る。稲垣（A03 計画）は、細胞接着分子 L1-CAM が細胞膜上で軸索を伸ばすための推進力を伝えるタイヤのような働きをすることを見出し、細胞と細胞外環境の間に生じる力と分子の滑りを巧妙に利用した新たな走触性の仕組みを明らかとした。稲垣と水野（A03 公募）は、既知のモータータンパク質による輸送とは異なる新しい細胞内分子輸送機構を明らかとした。

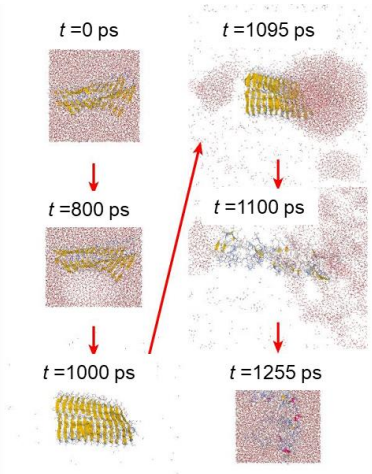
糖鎖の 3 次元構造ダイナミクスが展開する仕組みを解明

主な発表論文：*Sci. Rep.* 2017【A03 岡本、A03 加藤の共同】、*Adv. Exp. Med. Biol.* 2015【A02 神谷、A03 岡本、A03 加藤の共同】、*J. Cell Biol.* 2015【A02 神谷、A03 加藤の共同】

細胞内で新たに作られたタンパク質が小胞体において立体構造を形成する際や、固有の立体構造獲得後にゴルジ体へと移る際、あるいは不要となったタンパク質が分解処理されるプロセスには、糖鎖をはじめとする多数の生命分子素子が関与している。岡本（A03 計画）は、レプリカ交換分子動力学シミュレーションによって、複雑な分岐構造を有するオリゴ糖鎖の配座空間を探査した。こうした理論的アプローチに、加藤（A03 計画）が開発してきた常磁性 NMR 法による精密実験データを組み合わせることにより、輸送や分解といったタンパク質の運命を規定する糖鎖の立体構造のダイナミクスや、タンパク質によって糖鎖が認識されるプロセスを明らかにすることに成功した。

アミロイド線維の形成と崩壊の過程を捉えた

主な発表論文：*J. Phys. Chem. B* 2016【A03 奥村】、*Sci. Rep.* 2015【A03 茶谷、A03 杉山の共同】



奥村（A03 公募）は、独自開発したハミルトニアンレプリカ置換分子動力学計算手法により、アミロイド β ペプチドの線維化初期段階におけるシミュレーションを行い、分子間 β シート構造形成による 2 量体形成過程を観測することに成功した。さらに、外部刺激による線維破壊のメカニズムを明らかにするとともに、線維伸長の方向が制御されるメカニズムを解明した。さらに、茶谷と杉山（ともに A03 公募）の共同研究では、線維形成反応の開始に同期させた時分割小角 X 線散乱測定を実施し、タンパク質の初期集合体の形状や、徐々に肥大成長しながら成熟線維へと構造発達する様子を捉えることに成功した。

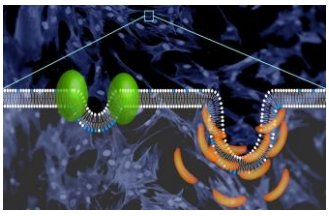
時計じかけの秩序形成の仕組みを解明

主な発表論文：*Sci. Rep.* 2016【A03 加藤、A03 内山、A03 杉山、A03 寺内の共同】、*Science* 2015【A01 秋山(修)】

ATP の結合と加水分解に共役してダイナミックな離合集散を伴うシアノバクテリア時計タンパク質の作動原理も明らかとなりつつある。秋山(修)（A01 公募）は、ATP の加水分解にはペプチド主鎖の異性化反応を伴った大規模な構造転移、24 時間周期の遅いリズムの根源が KaiC の構造の中にプログラムされていることを明らかとした。A03 班の複数のグループの共同研究（寺内、杉山、内山、加藤）では、未変性質量分析および中性子小角散乱を利用して KaiB-KaiC タンパク質複合体の化学量論数決定と複合体を構成するサブユニットの空間配置情報を明らかにした。

生体膜の動的秩序と膜タンパク質の離合集散動態の解明

主な発表論文：*Nature Commun.* 2017【A03 申】、*Sci. Rep.* 2017 【A01 松森、A03 老木の共同】、*J. Phys. Chem. Lett.* 2017【A01 内橋、A03 老木の共同】



申（A03 公募）は、シグナル依存的なフリッパーゼの活性調節メカニズムを解明し、細胞膜脂質 2 重層でのリン脂質非対称性を維持するシステムが解明された。脂質 2 重層間のリン脂質の移動（フリップ・フロップ）によって細胞膜の曲率形成を駆動することを明らかにした。老木（A03 公募）は、松森や内橋（ともに A01 公募）との連携によりイオンチャネルのゲーティングに伴って膜中で集合離散する動態を初めて明らかにした。