Kakenhi tips for young researchers

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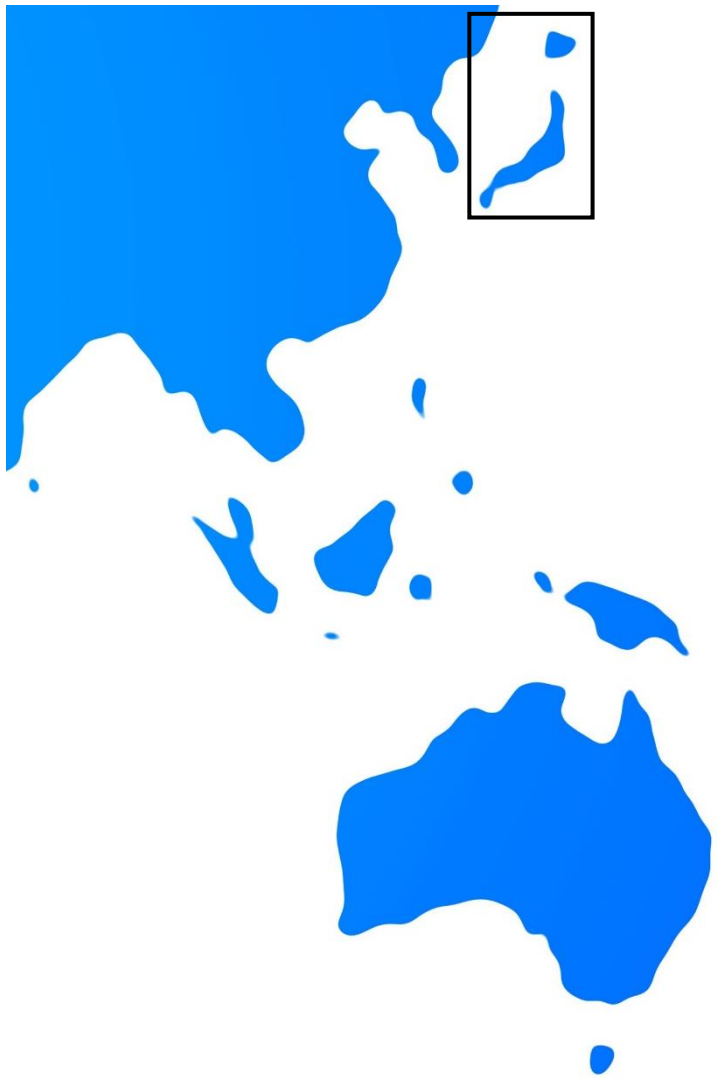
京都大学
KYOTO UNIVERSITY

Self-introduction

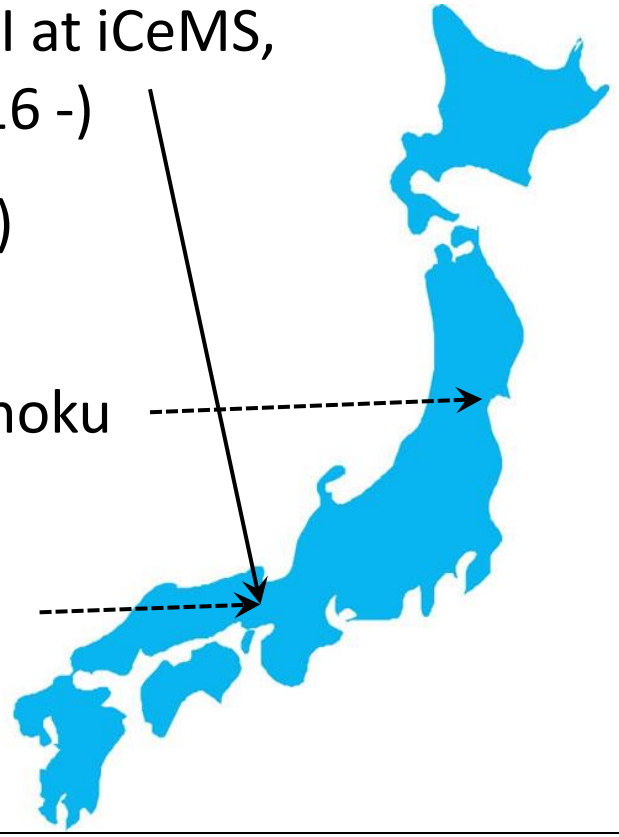


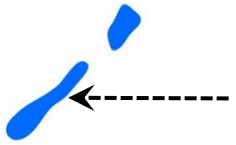
Senior lecturer and PI at iCeMS,
Kyoto University (2016 -)

JST PRESTO (Collaborative Math)
(2014 – 2018)

Assistant Professor at Tohoku University (2012 – 2016)

JSPS Postdoc at Kyoto University
Graduate School of Science
（2010-2012）





University of Canterbury (PhD 2010)
Major: Chemistry, Minor: Statistics

Why obtain research grants?

As well as paying for your research costs, research grants show that

- you have a **sound long-term research plan**,
- that people believe your **research will yield exciting outcomes**, and
- that you have the **support of the domestic community**.

It is very hard to demonstrate these things from your publication record alone.

Kakenhi is the main source of public research funding in Japan

Main categories:	**Target age:**
Kiban S	50 onwards
Kiban A	Mid 40s onwards
Kiban B	Late 30s – late 40s
Kiban C	Mid 30s – early 40s
Wakate (Young Scientists)	Late 20s – late 30s

(+ other special categories)

As you go through your career, you work your way up from Wakate to Kiban S.

My mixed Kakenhi history…

Occasional hits!

2014: Young researchers B (Wakate B)
Charge transport inside of organic crystals

2016: Shingakujyutsu Koubo
Nanostructure control with Bayesian optimisation

2018: Young researchers (Wakate)
Thin-film deposition system combining experiment and information science

2020: Kiban C
Quantum annealing for functional molecular assemblies

+ others!

Occasional misses!

2017: Challenging Research (Chosentekihouga)
Molecular transport network based upon a mathematical model

2017: Young researcher A (Wakate A)
Computational platform for work function control

2018: Shingakujyutsu Koubo
Determination of nanopore atomic structure via a math-materials collaboration

2019: Kiban B
Molecular assembly control by fusion of computation and machine learning

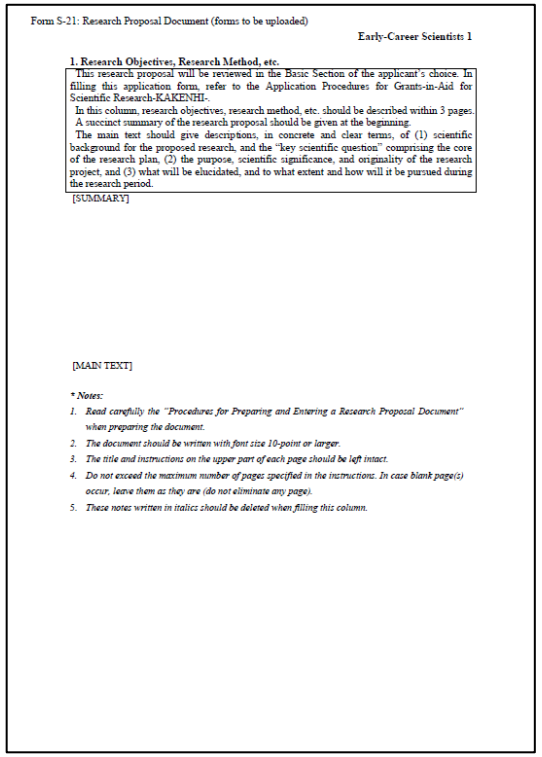
+ others!

All established researchers have a long list of acceptance and rejections.

If you miss once, just re-think your strategy and try again.

What do you need to write?

Wakate application form: https://www.jsps.go.jp/english/e-grants/data/r02/s-21_e.doc



Form S-21: Research Proposal Document (forms to be uploaded)

Early-Career Scientists 1

1. Research Objectives, Research Method, etc.

This research proposal will be reviewed in the Basic Section of the applicant's choice. In filling this application form, refer to the Application Procedures for Grants-in-Aid for Scientific Research-KAKENHI-.

In this column, research objectives, research method, etc. should be described within 3 pages.

A succinct summary of the research proposal should be given at the beginning.

The main text should give descriptions, in concrete and clear terms, of (1) scientific background for the proposed research, and the "key scientific question" comprising the core of the research plan, (2) the purpose, scientific significance, and originality of the research project, and (3) what will be elucidated, and to what extent and how will it be pursued during the research period.

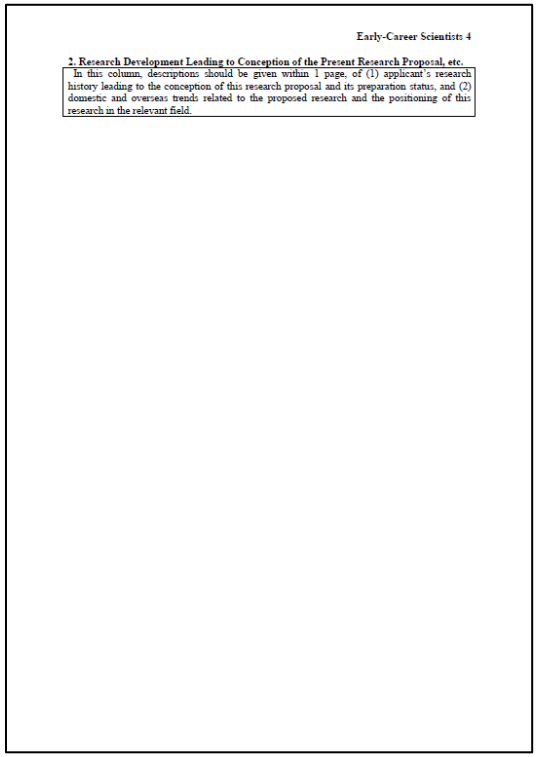
[SUMMARY]

[MAIN TEXT]

** Notes:*

1. *Read carefully the "Procedures for Preparing and Entering a Research Proposal Document" when preparing the document.*
2. *The document should be written with font size 10-point or larger.*
3. *The title and instructions on the upper part of each page should be left intact.*
4. *Do not exceed the maximum number of pages specified in the instructions. In case blank page(s) occur, leave them as they are (do not eliminate any page).*
5. *These notes written in italics should be deleted when filling this column.*

Proposal:
Summary, goal, methods (3 pages)

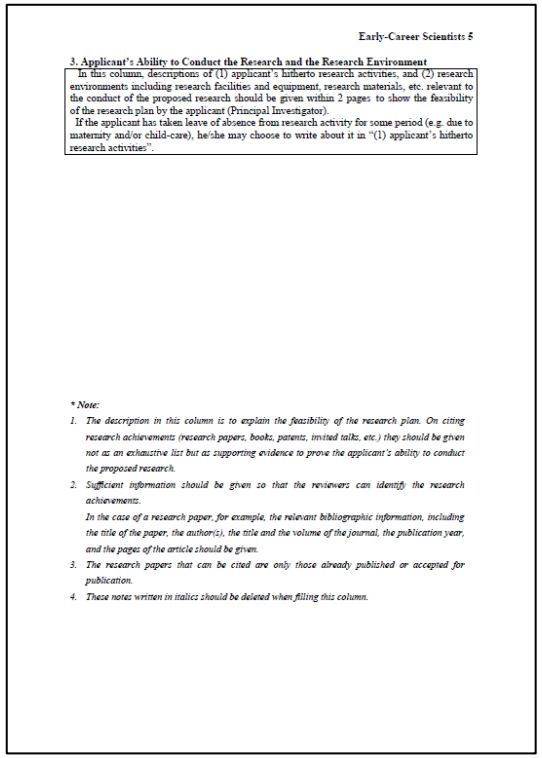


Early-Career Scientists 4

2. Research Development Leading to Conception of the Present Research Proposal, etc.

In this column, descriptions should be given within 1 page, of (1) applicant's research history leading to the conception of this research proposal and its preparation status, and (2) domestic and overseas trends related to the proposed research and the positioning of this research in the relevant field.

Background:
How did you choose this project? (1 page)



Early-Career Scientists 5

3. Applicant's Ability to Conduct the Research and the Research Environment

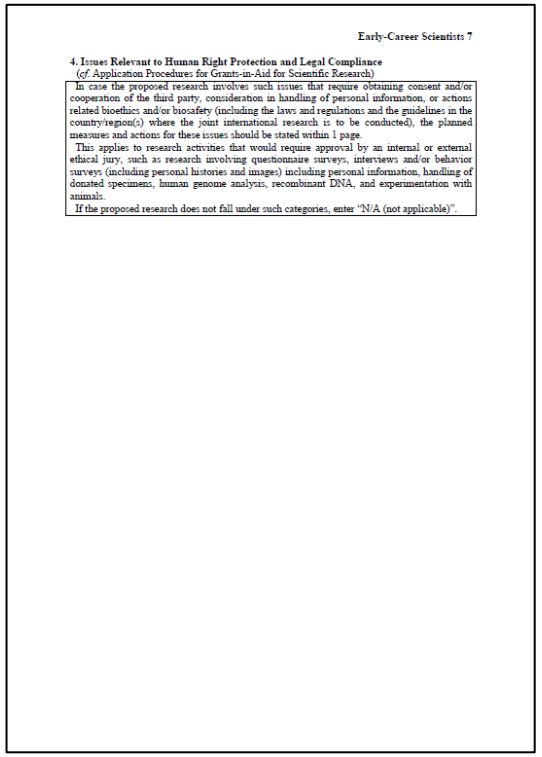
In this column, descriptions of (1) applicant's hitherto research activities, and (2) research environments including research facilities and equipment, research materials, etc. relevant to the conduct of the proposed research should be given within 2 pages to show the feasibility of the research plan by the applicant (Principal Investigator).

If the applicant has taken leave of absence from research activity for some period (e.g. due to maternity and/or child-care), he/she may choose to write about it in "(1) applicant's hitherto research activities".

** Note:*

1. *The description in this column is to explain the feasibility of the research plan. On citing research achievements (research papers, books, patents, invited talks, etc.) they should be given not as an exhaustive list but as supporting evidence to prove the applicant's ability to conduct the proposed research.*
2. *Sufficient information should be given so that the reviewers can identify the research achievements.*
   In the case of a research paper, for example, the relevant bibliographic information, including the title of the paper, the author(s), the title and the volume of the journal, the publication year, and the pages of the article should be given.
3. *The research papers that can be cited are only those already published or accepted for publication.*
4. *These notes written in italics should be deleted when filling this column.*

Feasibility:
Past achievements and current research environment (2 pages)



Early-Career Scientists 7

4. Issues Relevant to Human Right Protection and Legal Compliance

(*cf.* Application Procedures for Grants-in-Aid for Scientific Research)

In case the proposed research involves such issues that require obtaining consent and/or cooperation of the third party, consideration in handling of personal information, or actions related bioethics and/or biosafety (including the laws and regulations and the guidelines in the country/region(s) where the joint international research is to be conducted), the planned measures and actions for these issues should be stated within 1 page.

This applies to research activities that would require approval by an internal or external ethical jury, such as research involving questionnaire surveys, interviews and/or behavior surveys (including personal histories and images) including personal information, handling of donated specimens, human genome analysis, recombinant DNA, and experimentation with animals.

If the proposed research does not fall under such categories, enter "N/A (not applicable)".

Compliance:
Human rights protections, etc (1 page)

Elephant in the room….

https://dotunadeoye.com/2019/09/18/whos-the-elephant-in-your-business-idea-room/

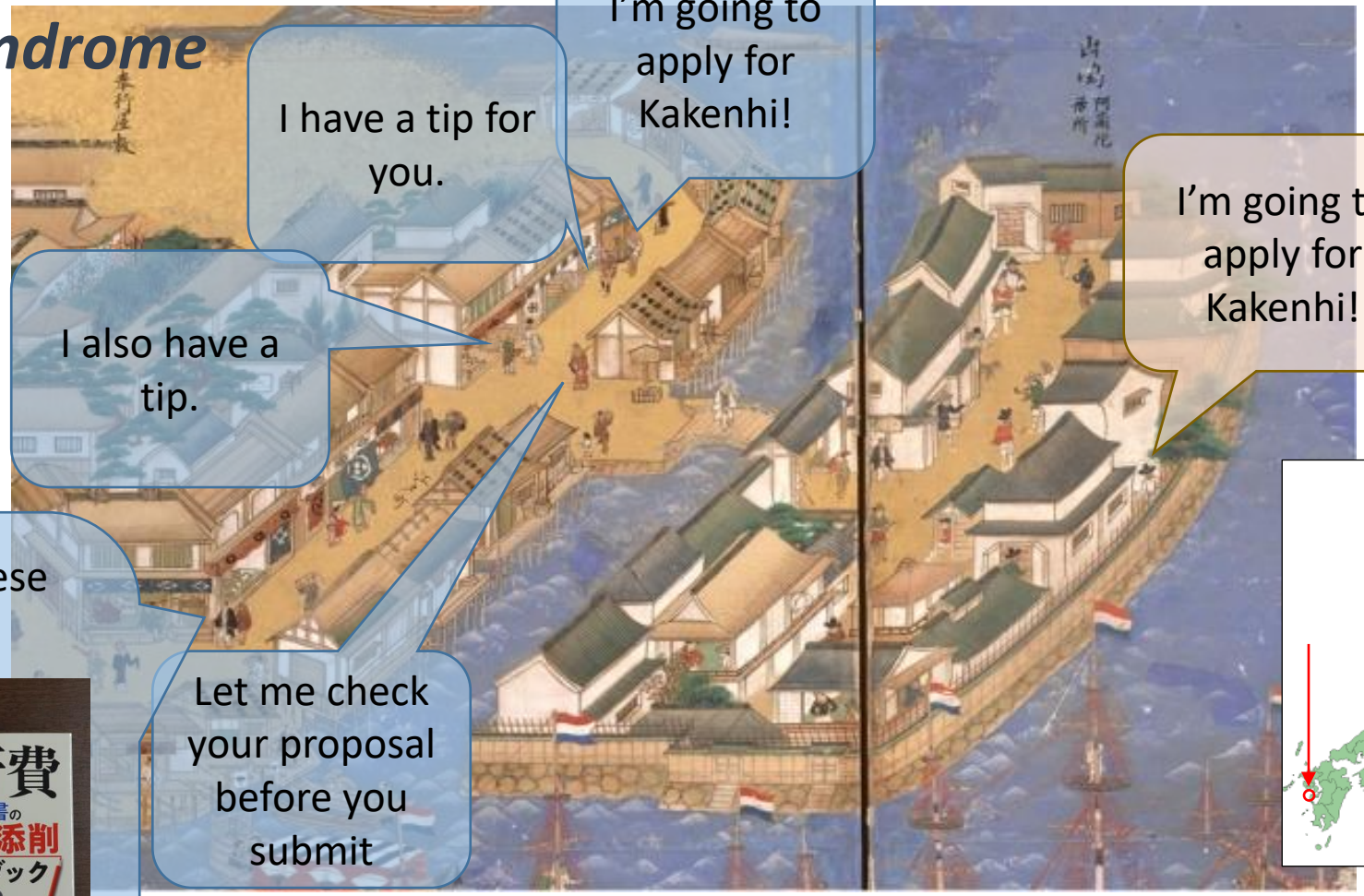
	2013 success rate for Japanese proposals	English proposals
Kiban A	23.5 %	13.6 %
Kiban B	24.7 %	11.4 %
Kiban C	29.9 %	23.7 %
Challenging (houga)	25.8 %	10.9 %
Wakate A	22.1 %	9.8 %
Wakate B	29.9 %	20.0 %

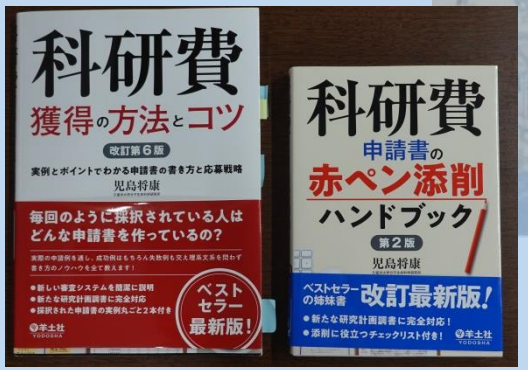
http://www.mext.go.jp/b_menu/shingi/gijyutu/gijyutu4/037/shiryo/__icsFiles/afieldfile/2015/06/17/1358876_05.pdf

A contributing factor:

Dejima syndrome

https://keijoseph.amebaownd.com/posts/10760934/





Nowadays, anybody can roam Japan freely. The tangible parts of Japan are fully accessible.

However, the intangible parts (information) remain somewhat inaccessible.

8 tips (that I am confident about)

2 tips (that I am less confident about)

Tip # 1: Remember that the evaluators are really busy!

https://ex02.net/archives/23

様式Ｓ－８（応募内容ファイル（添付ファイル項目））

新学術（公募）－１

研究概要

（１）研究目的等

新学術（公募）－２、３（研究目的）、６（今回の研究計画を実施するに当たっての準備状況及び研究成果を社会・国民に発信する方法）、７（これまでに受けた研究費とその成果等）、８（前回の公募研究の成果等）の内容を簡潔にまとめて記述してください。（1/2 頁程度、「研究計画・方法」と合わせて１頁以内）

Nanoporous metals display exceptional catalytic activity for a variety of chemical reactions. In this research, we will **elucidate the atomic-scale structure of nanoporous metals *via* interdisciplinary mathematics-materials science research**. Then, by correlating structure with catalytic activity, we will **elucidate the relationship between atomic-scale structure and catalytic activity.**

We will use small molecules as probes for the atomic-scale structure of nanoporous metals (Fig 1). In the *mathematics* part of our study, we will create a model for the structures of the pore walls. In the *materials science* part, we will deposit probe molecules onto the pore walls and measure their infrared (vibrational) spectra. By interpreting the spectra with the model, we will obtain the pore wall atomic structure. By fitting catalytic activities to the atomic structures, we will then establish a relationship between catalytic activity and nanopore atomic structure.

- ***Problem*** Elucidation of atomic-scale structure of nanoporous metals
- ***Solution*** Use small molecules as probes for the nanoporous metal structure
- ***Mathematics*** Create a new model and Markov chain theory based on random diffeomorphisms to a surface.
- ***Materials science*** Deposit molecules onto real nanoporous metals, use infrared spectroscopy and math model to get atomic-scale structure
- ***Contribution to Ryoiki*** Act as a bridge between math and materials and facilitate interdisciplinary collaboration.

（２）研究計画・方法

新学術（公募）－４、５（研究計画・方法）の内容を簡潔にまとめて記述してください。（1/2 頁程度、「研究目的等」と合わせて１頁以内）

Mathematics: By incorporating surface deformation into our GAMMA model (*Nat. Commun.* **8**, 2017, 14463), we will create a new model for the possible structures of the pore walls inside of nanoporous metals. To predict the structures of the pore walls where the probe molecules adsorb, we will solve the model *via* a new theory for **Markov chains on spaces of deformed surfaces in $\mathbb{R}^3$**. By establishing a correspondence between these surfaces and atomic structure, the pore wall atomic structure can be predicted by simulating this Markov chain.

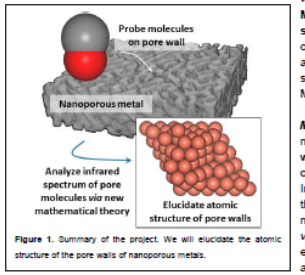
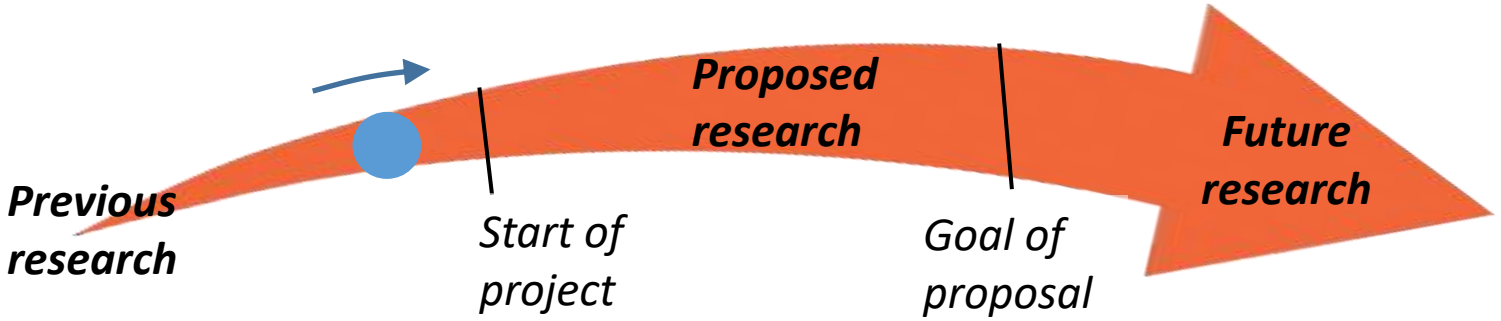


Figure 1. Summary of the project. We will elucidate the atomic structure of the pore walls of nanoporous metals.

Materials science: Real nanoporous metals will be created and probe molecules will be deposited onto their surfaces, using our ultra-high vacuum deposition system. Infrared (IR) spectroscopy will then measure the infrared (vibrational) spectra of probe molecules. By analyzing the infrared spectra *via* the mathematical theory above, we will elucidate the structure of the pore walls with atomic precision.

Make your proposal **interesting and easy-to-understand** for the evaluator.

Tip # 2: Before starting, think about where you have been and where you are going



- Successful proposals often feel like a chapter from a longer, personal story.
- Think about how your previous research brought you to the proposed project. Think about how the proposed project will bring you to your future research.
- This will help you to write with purpose and direction.

Early-Career Scientists 4

2. Research Development Leading to Conception of the Present Research Proposal, etc.

In this column, descriptions should be given within 1 page, of (1) applicant's research history leading to the conception of this research proposal and its preparation status, and (2) domestic and overseas trends related to the proposed research and the positioning of this research in the relevant field.

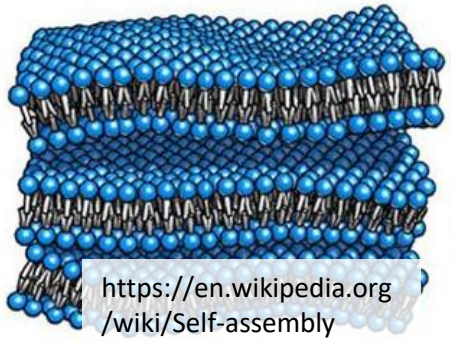
"…applicant's research history leading to the conception of this research proposal…"

Tip # 3: On the first page, articulate your vision and sell it

1. Big dream

Molecule

Self-assembly

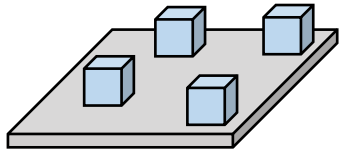


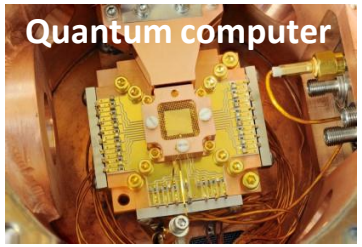
https://en.wikipedia.org/wiki/Self-assembly

Simulate the self-assembly process *within seconds* on a computer (impossible with ordinary computers)

2. This project (small version of the big dream)

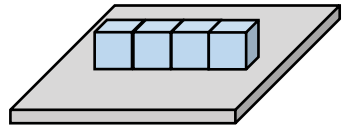
Molecule





https://algoanalytics.com/quantumAnnealers.html

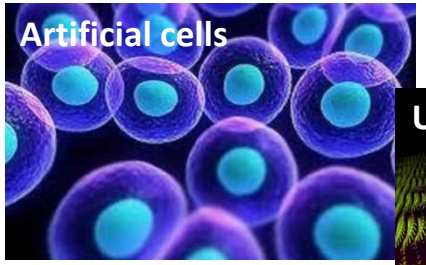
Self-assembly



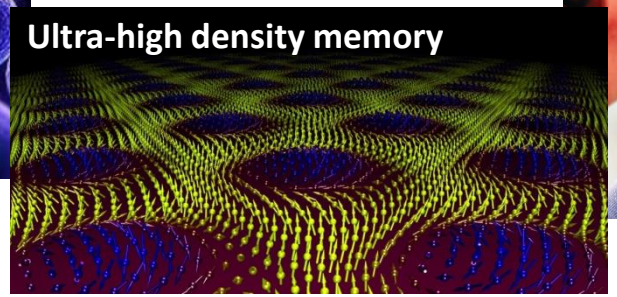
Simulate **on-surface** self-assembly using a **quantum computer**

3. Big impacts

Accelerate discovery of materials for future medicine and electronics



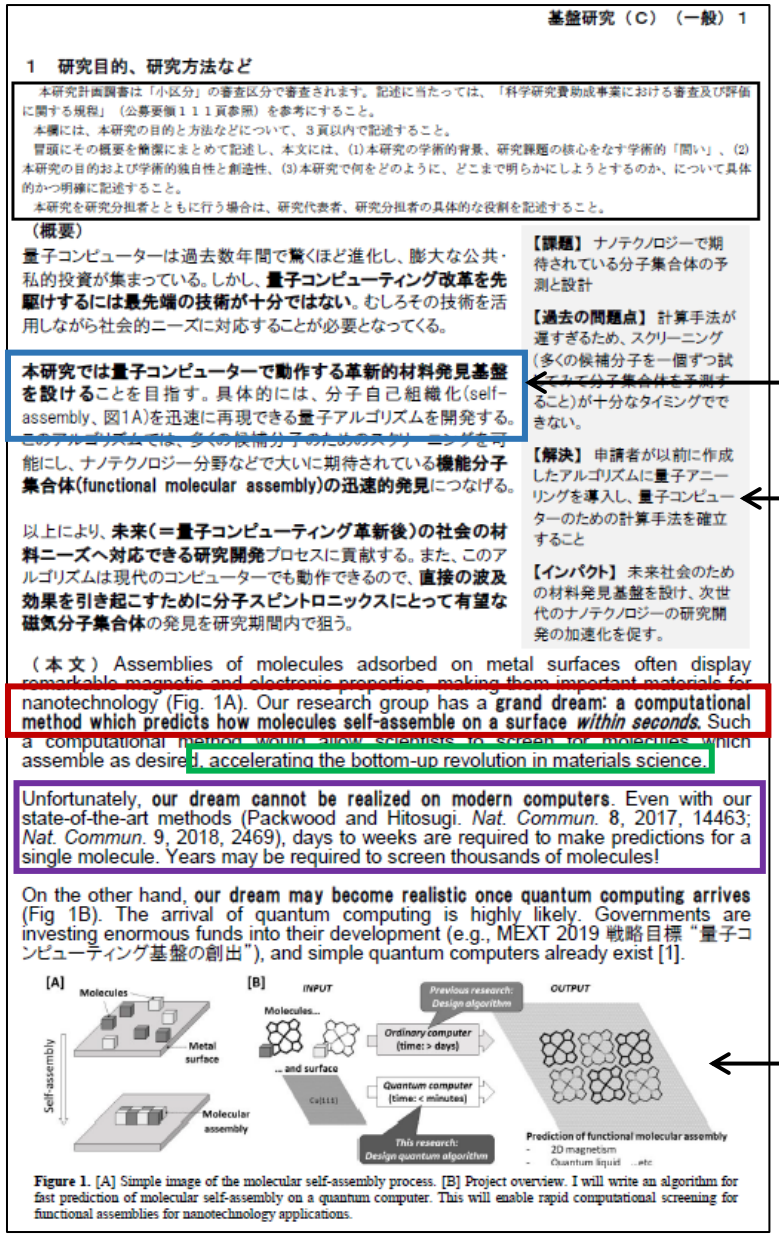
https://geneticliteracyproject.org/2018/11/14/creating-life-from-the-bottom-up-can-we-make-cells-from-scratch/



https://news.cnrs.fr/articles/the-new-challenges-of-spintronics

https://www.usatoday.com/story/tech/2014/03/20/reviewed-oled-tv-made-in-america/6568445/

Application form (first page)



基盤研究（C）（一般） 1

1　研究目的、研究方法など

本研究計画調書は「小区分」の審査区分で審査されます。記述に当たっては、「科学研究費助成事業における審査及び評価に関する規程」（公募要領１１１頁参照）を参考にすること。
本欄には、本研究の目的と方法などについて、３頁以内で記述すること。
冒頭にその概要を簡潔にまとめて記述し、本文には、(1)本研究の学術的背景、研究課題の核心をなす学術的「問い」、(2)本研究の目的および学術的独自性と創造性、(3)本研究で何をどのように、どこまで明らかにしようとするのか、について具体的かつ明確に記述すること。
本研究を研究分担者とともに行う場合は、研究代表者、研究分担者の具体的な役割を記述すること。

（概要）

量子コンピューターは過去数年間で驚くほど進化し、膨大な公共・私的投資が集まっている。しかし、**量子コンピューティング改革を先駆けするには最先端の技術が十分ではない**。むしろその技術を活用しながら社会的ニーズに対応することが必要となってくる。

本研究では量子コンピューターで動作する革新的材料発見基盤を設けることを目指す。具体的には、分子自己組織化(self-assembly、図1A)を迅速に再現できる量子アルゴリズムを開発する。このアルゴリズムでは、多くの候補分子のためのスクリーニングを可能にし、ナノテクノロジー分野などで大いに期待されている**機能分子集合体(functional molecular assembly)の迅速的発見**につなげる。

以上により、**未来(＝量子コンピューティング革新後)の社会の材料ニーズへ対応できる研究開発**プロセスに貢献する。また、このアルゴリズムは現代のコンピューターでも動作できるので、**直接の波及効果を引き起こすために分子スピントロニックスにとって有望な磁気分子集合体**の発見を研究期間内で狙う。

【課題】ナノテクノロジーで期待されている分子集合体の予測と設計

【過去の問題点】計算手法が遅すぎるため、スクリーニング（多くの候補分子を一個ずつ試してみて分子集合体を予測すること）が十分なタイミングでできない。

【解決】申請者が以前に作成したアルゴリズムに量子アニーリングを導入し、量子コンピューターのための計算手法を確立すること

【インパクト】未来社会のための材料発見基盤を設け、次世代のナノテクノロジーの研究開発の加速化を促す。

（本文）Assemblies of molecules adsorbed on metal surfaces often display remarkable magnetic and electronic properties, making them important materials for nanotechnology (Fig. 1A). Our research group has a **grand dream: a computational method which predicts how molecules self-assemble on a surface *within seconds***. Such a computational method would allow scientists to screen for molecules which assemble as desired, accelerating the bottom-up revolution in materials science.

Unfortunately, **our dream cannot be realized on modern computers**. Even with our state-of-the-art methods (Packwood and Hitosugi. *Nat. Commun.* 8, 2017, 14463; *Nat. Commun.* 9, 2018, 2469), days to weeks are required to make predictions for a single molecule. Years may be required to screen thousands of molecules!

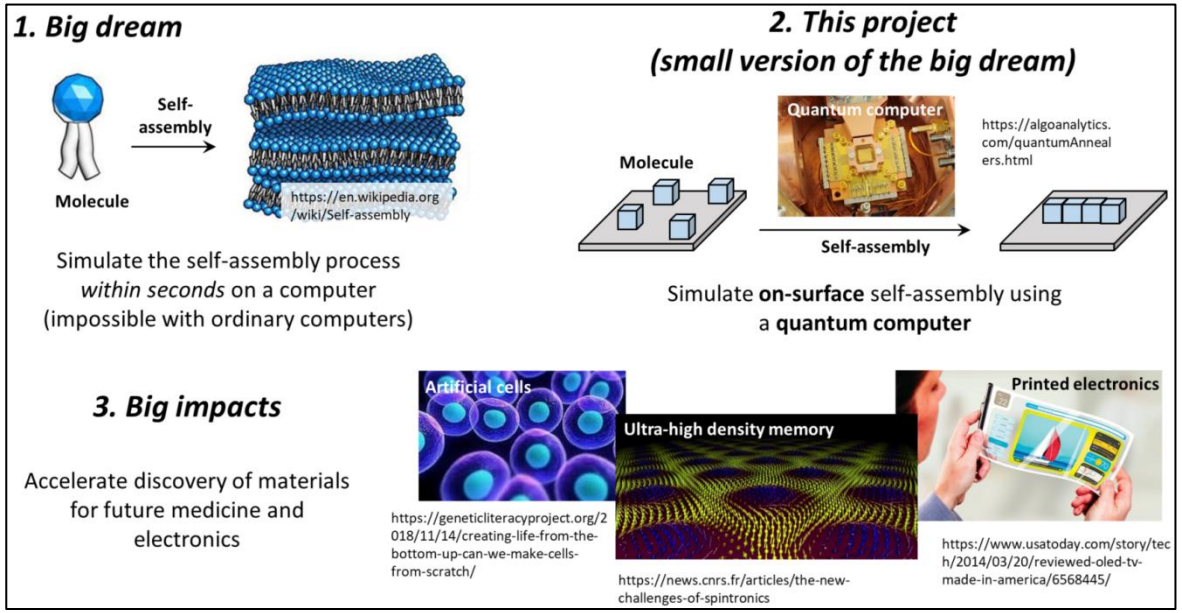
On the other hand, **our dream may become realistic once quantum computing arrives** (Fig 1B). The arrival of quantum computing is highly likely. Governments are investing enormous funds into their development (e.g., MEXT 2019 戦略目標 "量子コンピューティング基盤の創出"), and simple quantum computers already exist [1].

Figure 1. [A] Simple image of the molecular self-assembly process. [B] Project overview. I will write an algorithm for fast prediction of molecular self-assembly on a quantum computer. This will enable rapid computational screening for functional assemblies for nanotechnology applications.

Big dream

Impacts

Obstacle to big dream



This project + impacts

This research aims to lay-down a foundation for the discovery of novel materials [impacts] which runs on a quantum computer. More concretely, I will create an quantum algorithm which can quickly simulate on-surface self-assembly [this project].

Topic (big dream)**, problem** (obstacle to big dream)**, solution** (this project)**, impact**

This project + obstacle to big dream

Tip # 4: Make sure that flow of the project is clear at a glance

基盤研究（C）（一般）1

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（概要）

量子コンピューターは過去数年間で驚くほど進化し、膨大な公共・私的投資が集まっている。しかし、**量子コンピューティング改革を先駆けするには最先端の技術が十分ではない**。むしろその技術を活用しながら社会的ニーズに対応することが必要となってくる。

本研究では量子コンピューターで動作する革新的材料発見基盤を設けることを目指す。具体的には、分子自己組織化（self-assembly、図1A）を迅速に再現できる量子アルゴリズムを開発する。このアルゴリズムでは、多くの候補分子のためのスクリーニングを可能にし、ナノテクノロジー分野などで大いに期待されている**機能分子集合体(functional molecular assembly)の迅速的発見**につなげる。

以上により、**未来（＝量子コンピューティング革新後）の社会の材料ニーズへ対応できる研究開発**プロセスに貢献する。また、このアルゴリズムは現代のコンピューターでも動作できるので、**直接の波及効果を引き起こすために分子スピントロニックスにとって有望な磁気分子集合体**の発見を研究期間内で狙う。

【課題】ナノテクノロジーで期待されている分子集合体の予測と設計

【過去の問題点】計算手法が遅すぎるため、スクリーニング（多くの候補分子を一個ずつ試してみて分子集合体を予測すること）が十分なタイミングでできない。

【解決】申請者が以前に作成したアルゴリズムに量子アニーリングを導入し、量子コンピューターのための計算手法を確立すること

【インパクト】未来社会のための材料発見基盤を設け、次世代のナノテクノロジーの研究開発の加速化を促す。

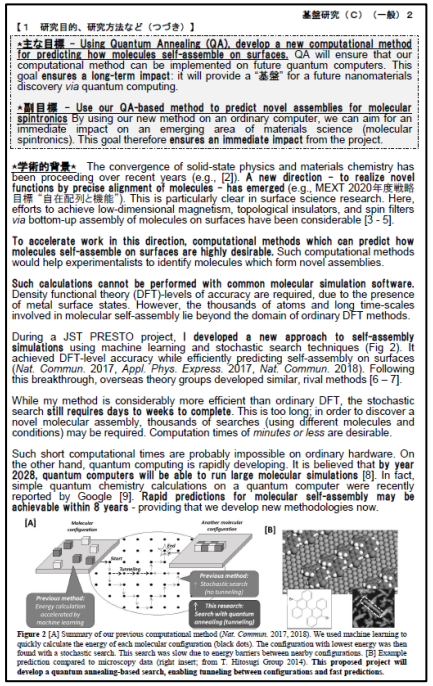
（本文）Assemblies of molecules adsorbed on metal surfaces often display remarkable magnetic and electronic properties, making them important materials for nanotechnology (Fig. 1A). Our research group has a **grand dream: a computational method which predicts how molecules self-assemble on a surface *within seconds***. Such a computational method would allow scientists to screen for molecules which assemble as desired, accelerating the bottom-up revolution in materials science.

Unfortunately, **our dream cannot be realized on modern computers**. Even with our state-of-the-art methods (Packwood and Hitosugi. *Nat. Commun.* 8, 2017, 14463; *Nat. Commun.* 9, 2018, 2469), days to weeks are required to make predictions for a single molecule. Years may be required to screen thousands of molecules!

On the other hand, **our dream may become realistic once quantum computing arrives** (Fig 1B). The arrival of quantum computing is highly likely. Governments are investing enormous funds into their development (e.g., MEXT 2019 戦略目標「量子コンピューティング基盤の創出」) and simple quantum computers already exist [1].

Figure 1. [A] Simple image of the molecular self-assembly process. [B] Project overview. I will write an algorithm for fast prediction of molecular self-assembly on a quantum computer. This will enable rapid computational screening for functional assemblies for nanotechnology applications.

Fig 1. Summary of project



基盤研究（C）（一般）2

【１　研究目的、研究方法など（つづき）】

★主な目標 – Using Quantum Annealing (QA), develop a new computational method for predicting how molecules self-assemble on surfaces. QA will ensure that our computational method can be implemented on future quantum computers. This goal **ensures a long-term impact**: it will provide a "**基盤**" for a future nanomaterials discovery *via* quantum computing.

★副目標 – Use our QA-based method to predict novel assemblies for molecular spintronics By using our new method on an ordinary computer, we can aim for an immediate impact on an emerging area of materials science (molecular spintronics). This goal therefore **ensures an immediate impact** from the project.

★学術的背景★ The convergence of solid-state physics and materials chemistry has been proceeding over recent years (e.g., [2]). **A new direction – to realize novel functions by precise alignment of molecules – has emerged** (e.g., MEXT 2020年度戦略目標「**自在配列化機能**」). This is particularly clear in surface science research. Here, efforts to achieve low-dimensional magnetism, topological insulators, and spin filters *via* bottom-up assembly of molecules on surfaces have been considerable [3 - 5].

To accelerate work in this direction, computational methods which can predict how molecules self-assemble on surfaces are highly desirable. Such computational methods would help experimentalists to identify molecules which form novel assemblies.

Such calculations cannot be performed with common molecular simulation software. Density functional theory (DFT)-levels of accuracy are required, due to the presence of metal surface states. However, the thousands of atoms and long time-scales involved in molecular self-assembly lie beyond the domain of ordinary DFT methods.

During a JST PRESTO project, **I developed a new approach to self-assembly simulations** using machine learning and stochastic search techniques (Fig 2). It achieved DFT-level accuracy while efficiently predicting self-assembly on surfaces (*Nat. Commun.* 2017, *Appl. Phys. Express.* 2017, *Nat. Commun.* 2018). Following this breakthrough, overseas theory groups developed similar, rival methods [6 – 7].

While my method is considerably more efficient than ordinary DFT, the stochastic search **still requires days to weeks to complete**. This is too long, in order to discover a novel molecular assembly, thousands of searches (using different molecules and conditions) may be required. Computation times of *minutes or less* are desirable.

Such short computational times are probably impossible on ordinary hardware. On the other hand, quantum computing is rapidly developing. It is believed that **by year 2028, quantum computers will be able to run large molecular simulations** [8]. In fact, simple quantum chemistry calculations on a quantum computer were recently reported by Google [9]. **Rapid predictions for molecular self-assembly may be achievable within 8 years** - providing that we develop new methodologies now.

Figure 2 [A] Summary of our previous computational method (*Nat. Commun.* 2017, 2018). We used machine learning to quickly calculate the energy of each molecular configuration (black dots). The configuration with lowest energy was then found with a stochastic search. This search was slow due to energy barriers between nearby configurations. [B] Example prediction compared to microscopy data (right inset; from T. Hitosugi Group 2014). **This proposed project will develop a quantum annealing-based search, enabling tunneling between configurations and fast prediction.**

Fig 2. Background / how this project overcomes previous bottlenecks

Fig 3. Method sketch
Fig 4. Immediate impact, long term impact

Fig 5 [because extra space was available] How to ensure immediate impact

Easy way: show one figure per page

The first figure should summarise the project (background, method, main goal).

Figures should be clear when printed in black-and-white!

【1　研究目的、研究方法など（つづき）】

⋆主な目標 – Using Quantum Annealing (QA), develop a new computational method for predicting how molecules self-assemble on surfaces. QA will ensure that our computational method can be implemented on future quantum computers. This goal **ensures a long-term impact**: it will provide a "基盤" for a future nanomaterials discovery *via* quantum computing.

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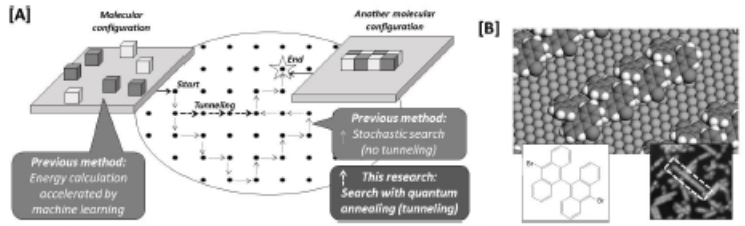

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Tip # 5: Write in short paragraphs

- Make one point per paragraph, use simple sentences
- **Key sentences in bold**. Proposal should be understandable by reading bold parts only. But do not use too much bold text.
- Have one line of space between paragraphs. This makes the proposal look easier to read.
- Avoid tiny font sizes. If you run out of space, you need write more succinctly.

Tip # 6: Plan to spend most of your time editing

https://www.brickcat.com/set-10662/

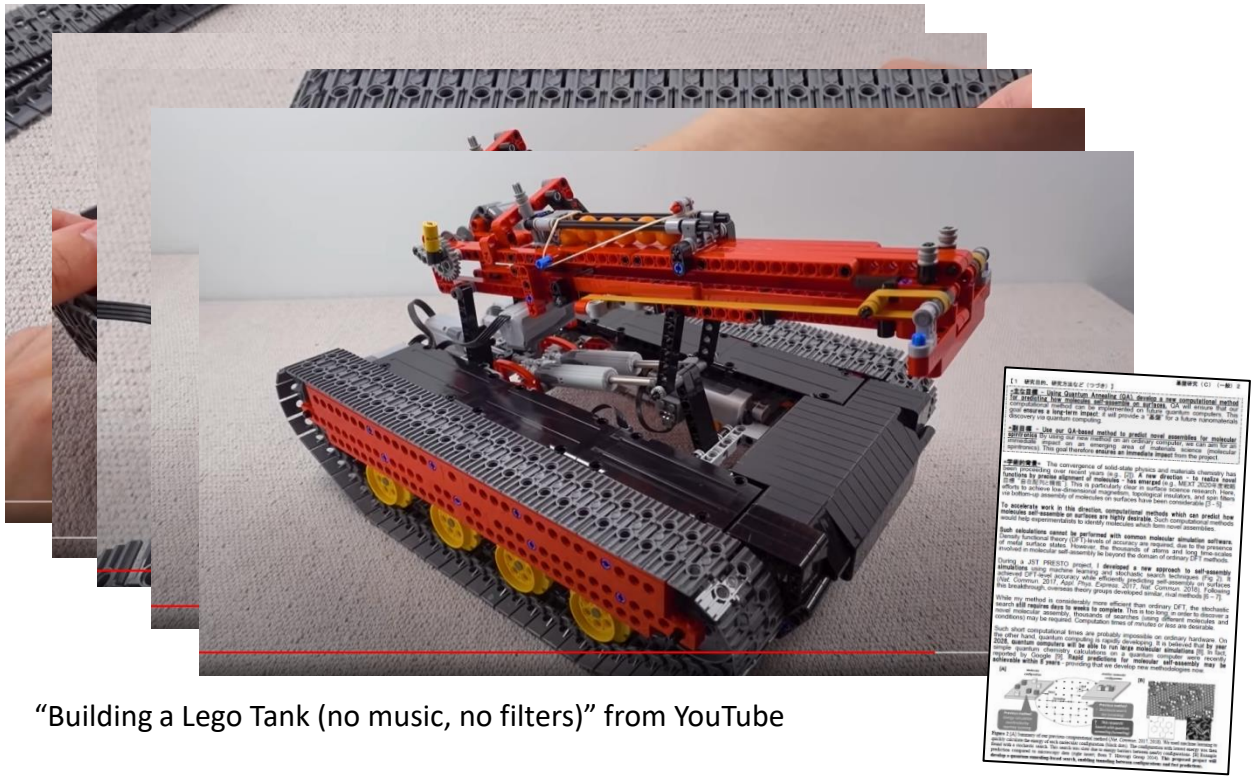
The convergence of solid-state physics and materials chemistry has been preceding over recent years. A new direction – to realise novel functionality by precise alignment of molecules – has emerged.

In previous research I developed a new approach to self-assembly simulations using machine learning and stochastic search techniques.

The database will be constructed from the Cambridge Online Crystal Database, which contains thousands of organic crystal structures.

Add →

← Remove



"Building a Lego Tank (no music, no filters)" from YouTube

- It is difficult to write the proposal from start to finish in one go. Because the space is quite limited (4 - 5 pages + figures), you will probably spend a lot of time editing.
- Efficient writing method: Write candidate paragraphs for each component of the project. Then, treat the candidate paragraphs like Lego plots. Click them together, remove some of them, add new ones, remove some more, etc, until you have the final proposal.

Tip # 7: Think carefully about which section you choose

Broad Section E		
Medium-sized Section 32: Physical chemistry, functional solid state chemistry, and related fields		
	Basic Section	
	32010	Fundamental physical chemistry-related
	32020	Functional solid state chemistry-related
Medium-sized Section 33: Organic chemistry and related fields		
	Basic Section	
	33010	Structural organic chemistry and physical organic chemistry-related
	33020	Synthetic organic chemistry-related
Medium-sized Section 34: Inorganic/coordination chemistry, analytical chemistry, and related fields		
	Basic Section	
	34010	Inorganic/coordination chemistry-related
	34020	Analytical chemistry-related
	34030	Green sustainable chemistry and environmental chemistry-related
Medium-sized Section 35: Polymers, organic materials, and related fields		
	Basic Section	
	35010	Polymer chemistry-related
	35020	Polymer materials-related
	35030	Organic functional materials-related

When you submit your proposal, you must select a 'section'.

Your proposal will be evaluated by senior researchers from that section.

Look through the entire list and choose appropriately!

List of fields:
https://www.jsps.go.jp/english/e-grants/data/2020/09/R2b_kouboyoryo_e.pdf

Tip # 8: Last but not least, familiarize yourself with E-rad!

- E-rad is the website where you submit your proposal.
- Access requires an ID and password. Your university administration provides this. Ask your secretary or office staff to obtain your ID and password from the administration.
- As well as uploading your proposal, you must enter additional information (amount of money required, etc). Check the submission page well ahead of the deadline.

https://www-shinsei.jsps.go.jp/kaken/index.html

8 tips (that I am confident about)

2 tips (that I am less confident about)

様式Ｓ－８（応募内容ファイル（添付ファイル項目））

新学術（公募）－１

研究概要

（１）研究目的等

新学術（公募）－２、３（研究目的）、６（今回の研究計画を実施するに当たっての準備状況及び研究成果を社会・国民に発信する方法）、７（これまでに受けた研究費とその成果等）、８（前回の公募研究の成果等）の内容を簡潔にまとめて記述すること。(1/2 頁程度、「研究計画・方法」と合わせて１頁以内)

・金属錯体の非対称性に基づく二次元磁性　第一原理構造予測で材料探索・

長距離磁気秩序を示す二次元材料はスピントロニクスのために非常に期待されている。本研究では、非対称金属錯体の自己組織化で形成した単一層を対象とし、第一原理から単一層の構造を予測できる手法（＝first-principles structure prediction およびFPSP コード）の開発を目指す（図 1A）。また、コードによるバーチャルスクリーニングを行い、長距離磁気秩序を示す単一層を形成できる金属錯体を探索する（図 1B）。

この探索を行うために、不対電子間の相互作用（強磁性相互作用、反強磁性相互作用）が電子間距離に依存することを活かす。具体的に、金属錯体の非対称性による単一層中の不対電子間距離に変異を導入し、新たなスピン配置を引き起こす。そして、非対称性を維持しながら金属錯体間相互作用を最適化して、長距離の強磁性・反強磁性を同時に示す単一層を形成できる金属錯体を絞り込む。

本研究では、前に作られたコード[*Nature Communications* 2017, 2018]をさらに発達し、不対電子・非対称性を有する金属錯体を取り扱うことで従来の第一原理構造予測と全く違う方向性へ進む。さらに、領域内の実験係共同研究者を見つけ、「配位アシンメトリー領域」へ積極的に貢献しながら材料科学実験へのフィードバックを狙う。

課題：長距離磁気秩序を示す金属錯体単一層の探索

解決：金属錯体単一層の構造を第一原理から予測できるコードを開発し、適当な単一層をバーチャルに探索すること

非対称性の出番：金属錯体の非対称性が単一層中の長距離磁気秩序を引き起こすこと

領域への貢献：配位アシンメトリーに基づく機能を発揮する材料を理論的に研究すること

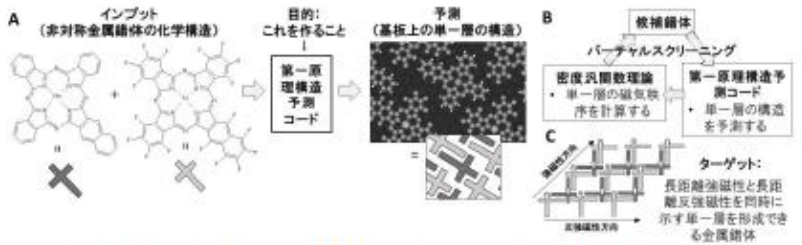


図 1. 本研究の目的・計画　(A)H31 年度は、非対称金属錯体の自己組織化で形成する単一層を対象とし、単一層の原子構造を予測できるコード(以下、FPSP コード)の開発を目指す。(B)H31 年度は、コードと密度汎関数理論によってバーチャルスクリーニングを行い、長距離磁気秩序を示す単一層を形成できる金属錯体の探索を目指す。(C)金属錯体の非対称性が引き起こす長距離磁気秩序の例。

（２）研究計画・方法

新学術（公募）－４、５（研究計画・方法）の内容を簡潔にまとめて記述すること。(1/2 頁程度、「研究目的等」と合わせて１頁以内)

平成 31 年度(図 1A)：FPSP コードを作成するには、金属錯体単一層のエネルギーを計算するための方法と単一層の平衡構造を計算できるモンテカルロ法が望ましい。パラメーターや単一層の候補構造がかなり多いので、円滑に進むために申請者の機械学習専門知識を活用する。具体的には、金属錯体の配置の例とそのエネルギーが記入されたデータベースを形成し、データベース中の相関をパラメーターフリー機械学習（＝カーネル型機械学習）で抽出する。この相関を活かすと単一層のエネルギーを迅速に計算するかつ、単一層の候補構造の数を劇的に減らすことが可能になる。以上により、単一層のエネルギーを計算するための方法と効率の良いモンテカルロ法へ同時に到達する。データベースを密度汎関数理論で形成するので、単一層の構造を第一原理計算とほぼ同じ精度で予測できると考えられる。

平成 32 年度(図 1B,C)：バーチャルスクリーニングを行うために、Fe や Mn を有する非対称ポルフィリン誘導体を候補錯体とする。そして、様々な候補錯体について FPSP コードで単一層の構造を予測し、単一層の磁気秩序を密度汎関数理論で計算する。ここではポルフィリン誘導体の化学構造と単一層の磁気秩序の相関を観察しながら、長距離磁気秩序を示す単一層を形成させる候補金属錯体を絞り込むように進める。

Maybe # 1: First page in Japanese?

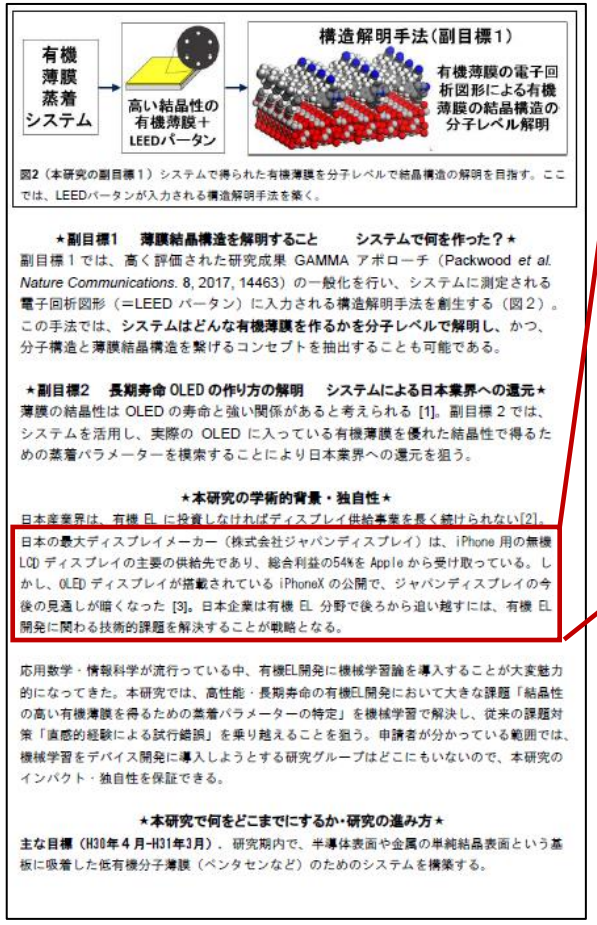
[Maybe] A good translation will improve the chances of success.

[Maybe not] A poor translation will do the opposite.

If a trusted colleague is available, do this with them and ask about the phrases they choose (helps if you can read Japanese).

Google Translator is not recommended.

Maybe # 2: Demonstrate knowledge of the real world



有機薄膜蒸着システム
高い結晶性の有機薄膜＋LEEDパターン
構造解明手法(副目標1)
有機薄膜の電子回析図形による有機薄膜の結晶構造の分子レベル解明

図2（本研究の副目標1）システムで得られた有機薄膜を分子レベルで結晶構造の解明を目指す。ここでは、LEEDパターンが入力される構造解明手法を築く。

★副目標1　薄膜結晶構造を解明すること　　システムで何を作った？★

副目標1では、高く評価された研究成果 GAMMA アポローチ（Packwood *et al. Nature Communications.* 8, 2017, 14463）の一般化を行い、システムに測定される電子回析図形（=LEED パターン）に入力される構造解明手法を創生する（図2）。この手法では、**システムはどんな有機薄膜を作るかを分子レベルで解明し**、かつ、分子構造と薄膜結晶構造を繋げるコンセプトを抽出することも可能である。

★副目標2　長期寿命 OLED の作り方の解明　　システムによる日本業界への還元★

薄膜の結晶性は OLED の寿命と強い関係があると考えられる [1]。副目標 2 では、システムを活用し、実際の OLED に入っている有機薄膜を優れた結晶性で得るための蒸着パラメーターを模索することにより日本業界への還元を狙う。

★本研究の学術的背景・独自性★

日本産業界は、有機 EL に投資しなければディスプレイ供給事業を長く続けられない[2]。

日本の最大ディスプレイメーカー（株式会社ジャパンディスプレイ）は、iPhone 用の無機 LCD ディスプレイの主要の供給先であり、総合利益の54%を Apple から受け取っている。しかし、OLED ディスプレイが搭載されている iPhoneX の公開で、ジャパンディスプレイの今後の見通しが暗くなった [3]。日本企業は有機 EL 分野で後ろから追い越すには、有機 EL 開発に関わる技術的課題を解決することが戦略となる。

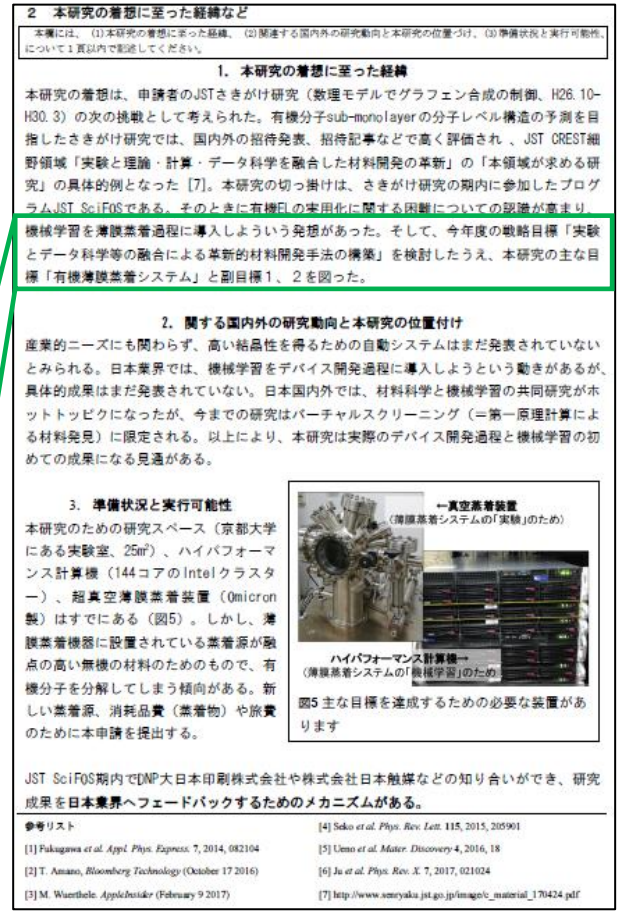
応用数学・情報科学が流行っている中、有機EL開発に機械学習論を導入することが大変魅力的になってきた。本研究では、高性能・長期寿命の有機EL開発において大きな課題「結晶性の高い有機薄膜を得るための蒸着パラメーターの特定」を機械学習で解決し、従来の課題対策「直感的経験による試行錯誤」を乗り越えることを狙う。申請者が分かっている範囲では、機械学習をデバイス開発に導入しようとする研究グループはどこにもいないので、本研究のインパクト・独自性を保証できる。

★本研究で何をどこまでにするか・研究の進め方★

主な目標（H30年4月-H31年3月）．研究期内で、半導体表面や金属の単純結晶表面という基板に吸着した低有機分子薄膜（ペンタセンなど）のためのシステムを構築する。

Japan's largest display maker (Japan Display) is the main producer of LCD displays for the iPhone, and receives 54 % of its total profit from Apple. However, with the announcement of the iPhoneX, which uses an OLED display, the future of Japan Display has become bleak.

Upon examining this year's Strategic Goals from MEXT (*New Material Development Method by Combination of Experiment and Data Science*), I formulated this project.



2　本研究の着想に至った経緯など

本欄には、（1）本研究の着想に至った経緯、（2）関連する国内外の研究動向と本研究の位置づけ、（3）準備状況と実行可能性、について1頁以内で記述してください。

1．本研究の着想に至った経緯

本研究の着想は、申請者のJSTさきがけ研究（数理モデルでグラフェン合成の制御、H26.10-H30.3）の次の挑戦として考えられた。有機分子sub-monolayerの分子レベル構造の予測を目指したさきがけ研究では、国内外の招待発表、招待記事などで高く評価され、JST CREST細野領域「実験と理論・計算・データ科学を融合した材料開発の革新」の「本領域が求める研究」の具体的例となった [7]。本研究の切っ掛けは、さきがけ研究の期内に参加したプログラムJST SciFOSである。そのときに有機ELの実用化に関する困難についての認識が高まり、機械学習を薄膜蒸着過程に導入しようという発想があった。そして、今年度の戦略目標「実験とデータ科学等の融合による革新的材料開発手法の構築」を検討したうえ、本研究の主な目標「有機薄膜蒸着システム」と副目標1、2を図った。

2．関する国内外の研究動向と本研究の位置付け

産業的ニーズにも関わらず、高い結晶性を得るための自動システムはまだ発表されていないとみられる。日本業界では、機械学習をデバイス開発過程に導入しようという動きがあるが、具体的成果はまだ発表されていない。日本国内外では、材料科学と機械学習の共同研究がホットトピックになったが、今までの研究はバーチャルスクリーニング（=第一原理計算による材料発見）に限定される。以上により、本研究は実際のデバイス開発過程と機械学習の初めての成果になる見通しがある。

3．準備状況と実行可能性

本研究のための研究スペース（京都大学にある実験室、25m²）、ハイパフォーマンス計算機（144コアのIntelクラスター）、超真空薄膜蒸着装置（Omicron製）はすでにある（図5）。しかし、薄膜蒸着機器に設置されている蒸着源が融点の高い無機の材料のためのもので、有機分子を分解してしまう傾向がある。新しい蒸着源、消耗品費（蒸着物）や旅費のために本申請を提出する。

←真空蒸着装置（薄膜蒸着システムの「実験」のため）
ハイパフォーマンス計算機→（薄膜蒸着システムの「機械学習」のため）

図5 主な目標を達成するための必要な装置があります

JST SciFOS期内でDNP大日本印刷株式会社や株式会社日本触媒などの知り合いができ、研究成果を**日本業界へフェードバックするためのメカニズムがある。**

参考リスト

[1] Fukugawa *et al. Appl. Phys. Express.* 7, 2014, 082104
[2] T. Amano, *Bloomberg Technology* (October 17 2016)
[3] M. Wuerthele. *Appleinsider* (February 9 2017)
[4] Seko *et al. Phys. Rev. Lett.* 115, 2015, 205901
[5] Ueno *et al. Mater. Discovery* 4, 2016, 18
[6] Ju *et al. Phys. Rev. X.* 7, 2017, 021024
[7] http://www.sanryaku.jst.go.jp/image/c_material_170424.pdf

[Maybe not] Kakenhi is meant for fundamental science.

[Maybe] For many evaluators, impact = solution to a 'real-world' problem

Final comments

基盤研究（C）（一般）1

1　研究目的、研究方法など

本研究計画調書は「小区分」の審査区分で審査されます。記述に当たっては、「科学研究費助成事業における審査及び評価に関する規程」（公募要領１１１頁参照）を参考にすること。
本欄には、本研究の目的と方法などについて、３頁以内で記述すること。
冒頭にその概要を簡潔にまとめて記述し、本文には、(1)本研究の学術的背景、研究課題の核心をなす学術的「問い」、(2)本研究の目的および学術的独自性と創造性、(3)本研究で何をどのように、どこまで明らかにしようとするのか、について具体的かつ明確に記述すること。
本研究を研究分担者とともに行う場合は、研究代表者、研究分担者の具体的な役割を記述すること。

（概要）

量子コンピューターは過去数年間で驚くほど進化し、膨大な公共・私的投資が集まっている。しかし、**量子コンピューティング改革を先駆けするには最先端の技術が十分ではない**。むしろその技術を活用しながら社会的ニーズに対応することが必要となってくる。

本研究では量子コンピューターで動作する革新的材料発見基盤を設けることを目指す。具体的には、分子自己組織化(self-assembly、図1A)を迅速に再現できる量子アルゴリズムを開発する。このアルゴリズムでは、多くの候補分子のためのスクリーニングを可能にし、ナノテクノロジー分野などで大いに期待されている**機能分子集合体(functional molecular assembly)の迅速的発見**につなげる。

以上により、**未来(＝量子コンピューティング革新後)の社会の材料ニーズへ対応できる研究開発**プロセスに貢献する。また、このアルゴリズムは現代のコンピューターでも動作できるので、**直接の波及効果を引き起こすために分子スピントロニックスにとって有望な磁気分子集合体**の発見を研究期間内で狙う。

【課題】ナノテクノロジーで期待されている分子集合体の予測と設計

【過去の問題点】計算手法が遅すぎるため、スクリーニング（多くの候補分子を一個ずつ試してみて分子集合体を予測すること）が十分なタイミングでできない。

【解決】申請者が以前に作成したアルゴリズムに量子アニーリングを導入し、量子コンピューターのための計算手法を確立すること

【インパクト】未来社会のための材料発見基盤を設け、次世代のナノテクノロジーの研究開発の加速化を促す。

（本文）Assemblies of molecules adsorbed on metal surfaces often display remarkable magnetic and electronic properties, making them important materials for nanotechnology (Fig. 1A). Our research group has a **grand dream: a computational method which predicts how molecules self-assemble on a surface *within seconds*.** Such a computational method would allow scientists to screen for molecules which assemble as desired, accelerating the bottom-up revolution in materials science.

Unfortunately, **our dream cannot be realized on modern computers**. Even with our state-of-the-art methods (Packwood and Hitosugi. *Nat. Commun.* 8, 2017, 14463; *Nat. Commun.* 9, 2018, 2469), days to weeks are required to make predictions for a single molecule. Years may be required to screen thousands of molecules!

On the other hand, **our dream may become realistic once quantum computing arrives** (Fig. 1B). The arrival of quantum computing is highly likely. Governments are investing enormous funds into their development (e.g., MEXT 2019 戦略目標 "量子コンピューティング基盤の創出"), and simple quantum computers already exist [1].

Figure 1. [A] Simple image of the molecular self-assembly process. [B] Project overview. I will write an algorithm for fast prediction of molecular self-assembly on a quantum computer. This will enable rapid computational screening for functional assemblies for nanotechnology applications.

- These tips are only based on my experience and do not guarantee success. You should take time to find what works for you.
- You should put a good effort into writing Kakenhi. It brings important career benefits and is a great chance to clarify your research direction.