Kakenhi tips for young researchers

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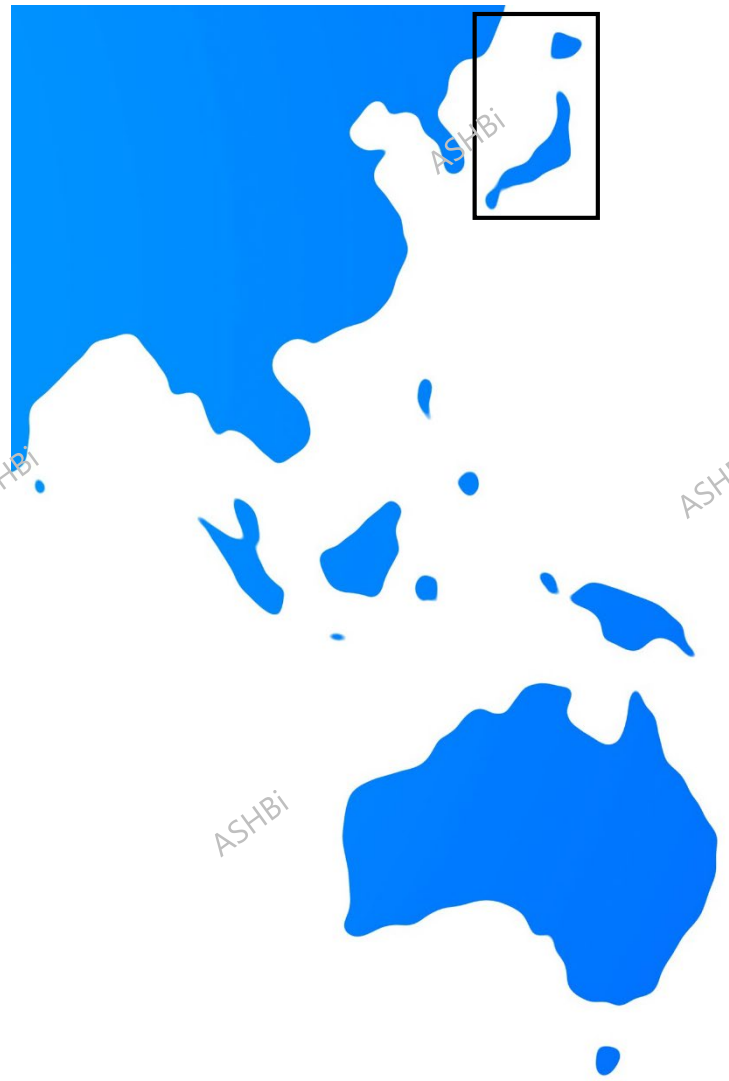
京都大学
KYOTO UNIVERSITY

Self-introduction

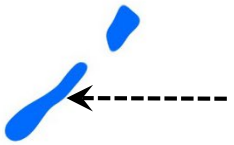


Senior lecturer and PI at iCeMS, Kyoto University (2016 -)

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 position:
Kiban S	Senior professor
Kiban A	Professor
Kiban B	Associate professor
Kiban C	Assistant / associate professor
Wakate (early career)	Postdoc / assistant professor

(+ 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

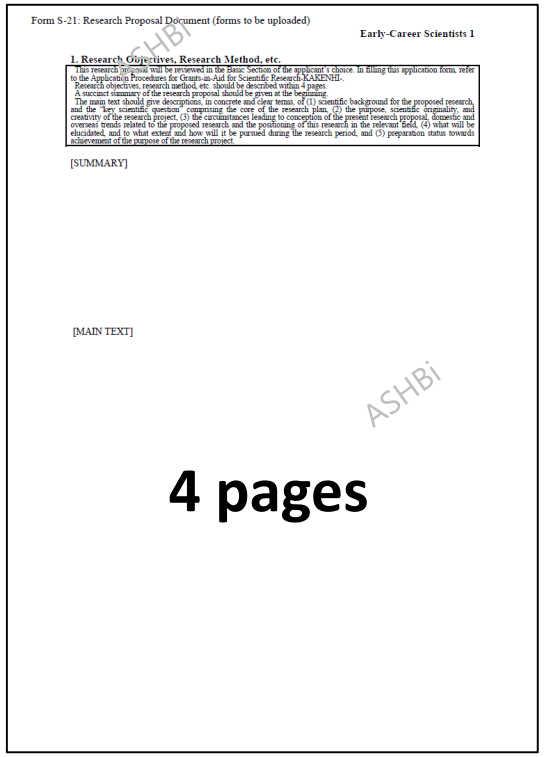
+ others!

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/j-grantsinaid/03_keikaku/data/r05/s-21.docx


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.

Research objectives, research method, etc. should be described within 4 pages.

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

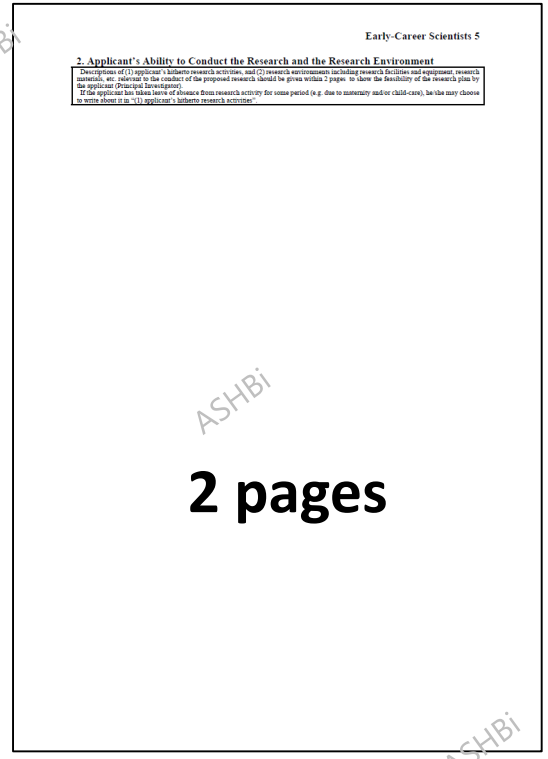
The main text should give descriptions, in concrete and clear terms, of (1) scientific background for the proposed research, and the "key scientific question" comprising the core of the research plan, (2) the purpose, scientific originality, and creativity of the research project, (3) the circumstances leading to conception of the present research proposal, domestic and overseas trends related to the proposed research and the positioning of this research in the relevant field, (4) what will be elucidated, and to what extent and how will it be pursued during the research period, and (5) preparation status towards achievement of the purpose of the research project.

[SUMMARY]

[MAIN TEXT]

4 pages

Proposal (main part):
Summary, goal, background, methods, how did you choose this project?


Early-Career Scientists 5

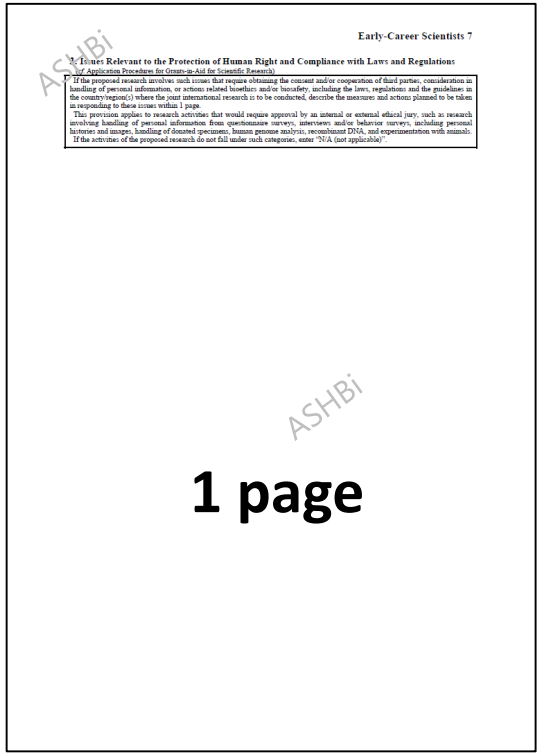
2. Applicant's Ability to Conduct the Research and the Research Environment

Descriptions of (1) applicant's hitherto research activities, and (2) research environment 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".

2 pages

Feasibility:
Past achievements and current research environment


Early-Career Scientists 7

3. Issues Relevant to the Protection of Human Right and Compliance with Laws and Regulations (cf. Application Procedures for Grants-in-Aid for Scientific Research).

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

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

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

1 page

Compliance:
Human rights protections, etc

Elephant in the room….

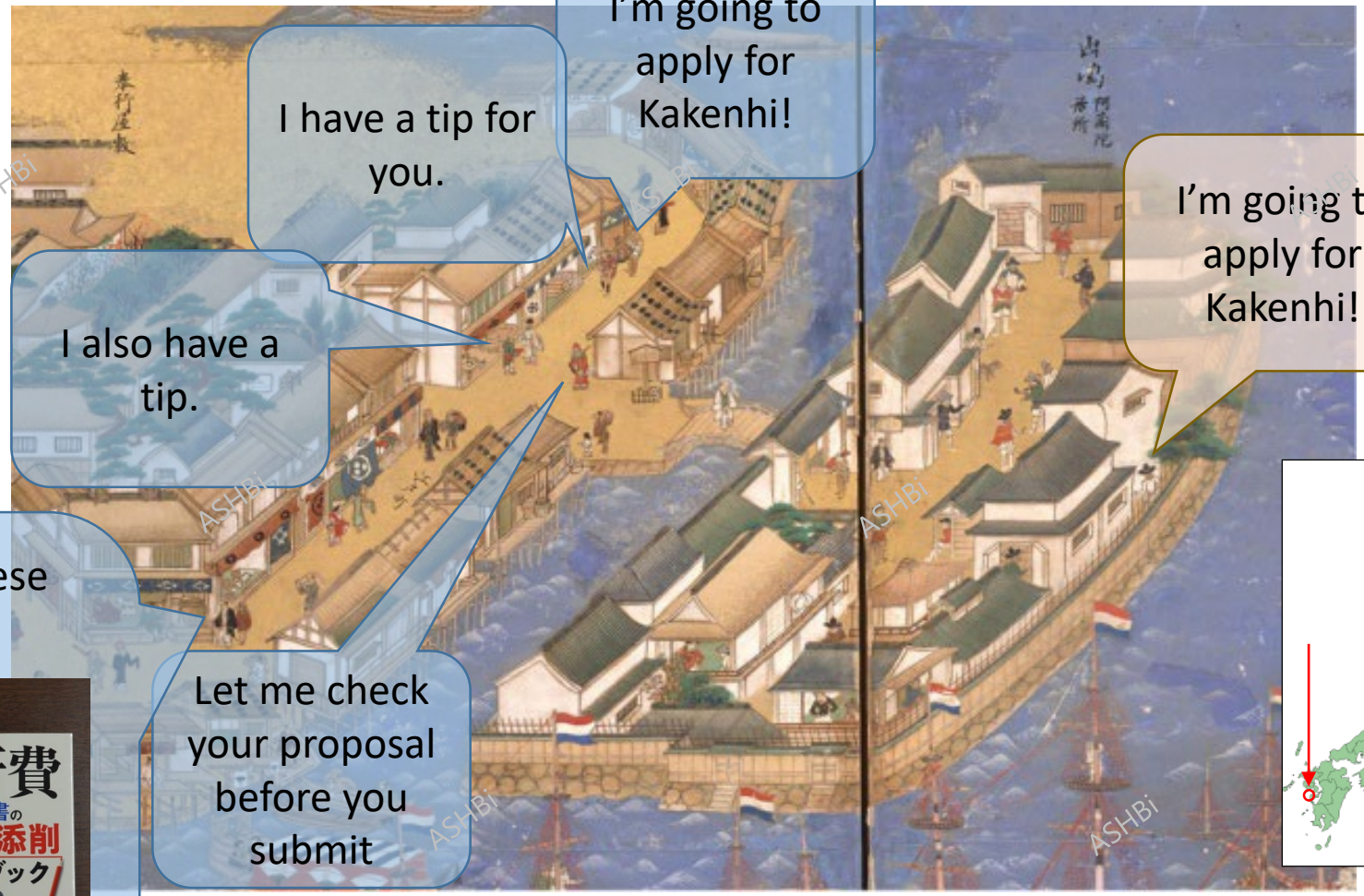
https://dotunadeoye.com/2019/09/18/whos-the-elephant-in-your-business-idea-room/

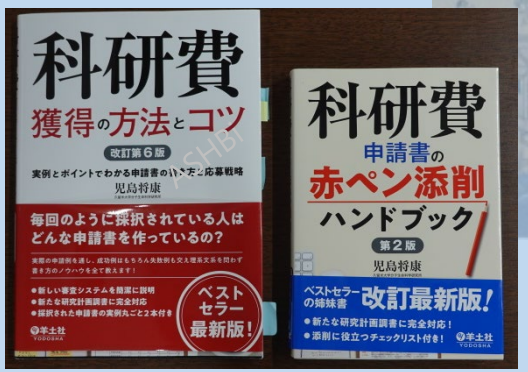
	2013 success rate for Japanese proposals	English proposals
Kiban A	23.5 %	13.6 %
Kiban B	24.7 %	11.4 %
Kiban C	29.9 %	23.7 %
Challenging (houga)	25.8 %	10.9 %
Wakate A	22.1 %	9.8 %
Wakate B	29.9 %	20.0 %

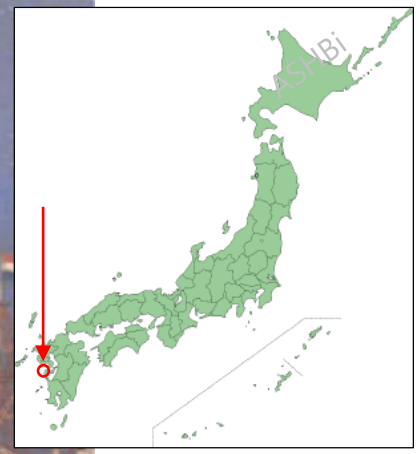
http://www.mext.go.jp/b_menu/shingi/gijyutu/gijyutu4/037/shiryo/__icsFiles/afieldfile/2015/06/17/1358876_05.pdf

Dejima syndrome?

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







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

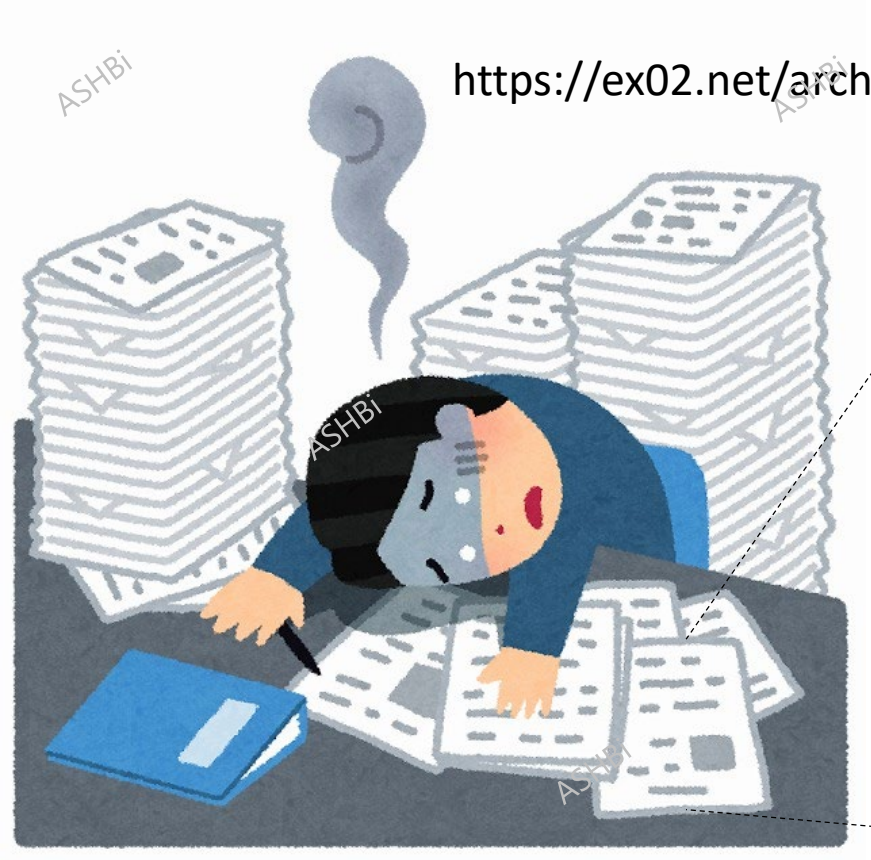
However, the intangible parts (information) remain inaccessible.

My Kakenhi tips!

Before you write

When you write

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（前回の公募研究の応募等）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.

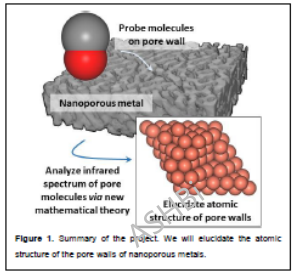


Figure 1. Summary of the project. We will elucidate the atomic structure of the pore walls of nanoporous metals.

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: Understand that you are not writing a paper

THE JOURNAL OF CHEMICAL PHYSICS 142, 144503 (2015)

Charge transport in organic crystals: Critical role of correlated fluctuations unveiled by analysis of Feynman diagrams

Daniel M. Packwood, Kazuaki Oniwa, Tienan Jin, and Naoki Asao
Advanced Institute for Materials Research, Tohoku University, Sendai, Japan

(Received 23 October 2014; accepted 18 March 2015; published online 9 April 2015)

Organic crystals have unique charge transport properties that lie somewhere between delocalised band-type transport and localised hopping transport. In this paper, we use a stochastic tight-binding model to explore how dynamical disorder in organic crystals affects charge transport. By analysing the model in terms of Feynman diagrams (virtual processes), we expose the crucial role of correlated dynamical disorder to the charge transport dynamics in the model at short times in the order of a few hundred femtoseconds. Under correlated dynamical disorder, the random motions of molecules in the crystal allow for low-energy "bonding"-type interactions between neighboring molecular orbitals can persist over long periods of time. On the other hand, the dependence of charge transport on correlated dynamical disorder also tends to localize the charge, as correlated disorder cannot persist far in space. This concept of correlation may be the "missing link" for describing the intermediate regime between band transport and hopping transport that occurs in organic crystals. © *2015 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4916385]

I. INTRODUCTION

Despite decades of intensive research, the nature of charge transport in high mobility organic crystals such as rubrene or pentacene remains controversial. In general, charge transport in organic crystals is characterised by two properties that are difficult to explain with conventional charge transport models,[1] namely, that near room temperature (a) electron and hole mobilities decrease in a power-law fashion with temperature[2] and (b) the mean free paths of electrons and holes are comparable to the crystal's unit cell size.[3] Property (a) is suggestive of delocalised band-type transport, with scattering by thermal molecular motions at higher temperature, whereas property (b) is suggestive of highly localised hopping transport between unit cells. Moreover, in the usual hopping transport picture, transport is activated by temperature. In order to reconcile these properties, simplified models with broad generality and mathematical analysis are extremely useful.

A long-established approach for studying temperature dependence of mobility in crystals is via polaron trapping of electrons (i.e., "local" electron-phonon interactions).[4] An important prediction of such theories is a crossover from band-type transport to hopping-type transport as temperature increases. For organic crystals, these theories explain property (b) well, however, they often run into difficulties in explaining (a). In more recent years, attention has turned to the large presence of *dynamical disorder* in organic crystals. This dynamical disorder, which arises from the erratic thermal motion of the molecules (inter-molecular phonon modes), is particularly conspicuous in organic crystals because the relatively weak van der Waals bonding between molecules allows for a large amount of molecular motion at room temperature.[5] The effect of dynamical disorder has been explored in recent years with a variety of theoretical approaches, including generalisations of the Holstein-Peierls model,[6–10] the hierarchy equations of motion,[11] and mixed quantum-classical models based on molecular dynamics or stochastic models of the molecular framework.[12–15] First principles calculations and molecular dynamics simulations have shown that the thermal molecular motions cause large modulation of the electronic coupling between molecules (i.e., "non-local electron-phonon" coupling) and dynamical localisation of charges.[17,18] This large modulation of the electronic coupling is due to the relatively large distances between adjacent molecules in the crystal and the complicated shape of the frontier orbitals of each molecule; small thermal motions of the molecules tend to produce erratic changes in both the sign and magnitude of the coupling.[17,18] This modulation could be considered as stochastic. At present, there appears to be a consensus in the literature that dynamical disorder and electron-phonon coupling are the central phenomena behind the charge transport properties (a) and (b). However, the unifying concept that underlies the calculation output and *connects* the dynamical disorder to charge transport mechanism in organic crystals has still not been highlighted.

In this paper, we study a tight-binding model with stochastic site-site coupling ("stochastic tight binding model"). This model is distinct from the widely studied Gaussian disorder models, which consider stochastic site energies.[19,20] While stochastic models can be used to model experimental data, they are especially convenient for exploring how intuitive concepts such as "correlation" and "amplitude" of the stochastic noise contribute to the model output. This latter quality of the stochastic models is of particular interest to the present paper. By a mathematical analysis of the stochastic tight-binding (STB) model, we identify a key set of Feynman diagrams that describe the charge transport physics. These Feynman diagrams highlight the central role of *correlated stochastic modulation* in the charge transport mechanism in the STB model. Correlated stochastic modulation means that under dynamical disorder, the relative orientation between molecular

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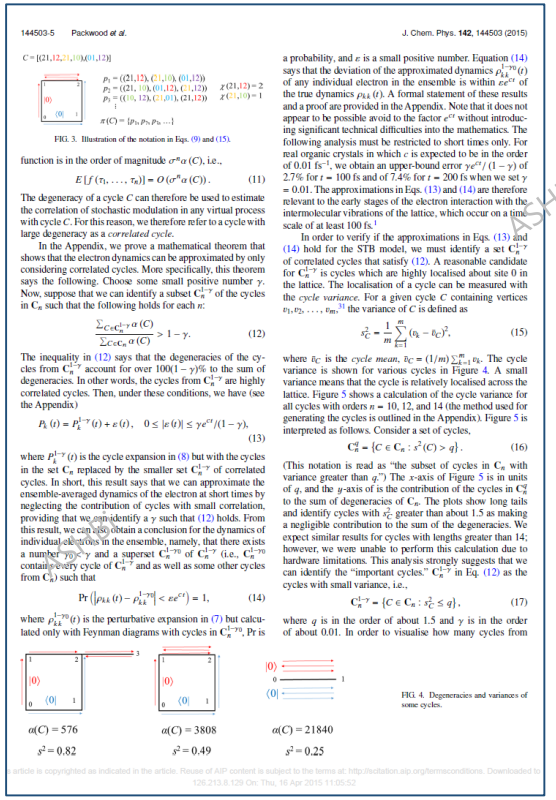

144503-5 Packwood *et al.* J. Chem. Phys. 142, 144503 (2015)

$C = [(21,12,\overline{21},\overline{10})(01,12)]$

$p_1 = ((21,12),(\overline{21},\overline{10}),(01,12))$
$p_2 = ((21,\overline{10}),(01,12),(\overline{21},12))$ $\chi(21,12) = 2$
$p_3 = ((\overline{10},12),(\overline{21},01),(21,12))$ $\chi(\overline{21},\overline{10}) = 1$
$\vdots$
$\pi(C) = [p_1, p_2, p_3, \ldots]$

FIG. 3. Illustration of the notation in Eqs. (9) and (15).

function is in the order of magnitude $\sigma^n \alpha(C)$, i.e.,

$$E\left[f(\tau_1, \ldots, \tau_K)\right] = O(\sigma^n \alpha(C)). \tag{11}$$

The degeneracy of a cycle C can therefore be used to estimate the correlation of stochastic modulation in any virtual process with cycle C. For this reason, we therefore refer to a cycle with large degeneracy as a *correlated cycle*.

In the Appendix, we prove a mathematical theorem that shows that the electron dynamics can be approximated by only considering correlated cycles. More specifically, this theorem says the following. Choose some small positive number γ. Now, suppose that we can identify a subset $\mathbf{C}_n^{1-\gamma}$ of the cycles in $\mathbf{C}_n$ such that the following holds for each n:

$$\frac{\sum_{C \in \mathbf{C}_n^{1-\gamma}} \alpha(C)}{\sum_{C \in \mathbf{C}_n} \alpha(C)} > 1 - \gamma. \tag{12}$$

The inequality in (12) says that the degeneracies of the cycles from $\mathbf{C}_n^{1-\gamma}$ account for over $100(1-\gamma)\%$ to the sum of degeneracies. In other words, the cycles from $\mathbf{C}_n^{1-\gamma}$ are highly correlated cycles. Then, under these conditions, we have (see the Appendix)

$$P_k(t) = P_k^{1-\gamma}(t) + \varepsilon(t), \quad 0 \le |\varepsilon(t)| \le \gamma e^{ct}/(1-\gamma), \tag{13}$$

where $P_k^{1-\gamma}(t)$ is the cycle expansion in (8) but with the cycles in the set $\mathbf{C}_n$ replaced by the smaller set $\mathbf{C}_n^{1-\gamma}$ of correlated cycles. In short, this result says that we can approximate the ensemble-averaged dynamics of the electron at short times by neglecting the contribution of cycles with small correlation, providing that we can identify a γ such that (12) holds. From this result, we can also obtain a conclusion for the dynamics of individual electrons in the ensemble, namely, that there exists a number $\gamma_0 > \gamma$ and a superset $\mathbf{C}_n^{1-\gamma_0}$ of $\mathbf{C}_n^{1-\gamma}$ (i.e., $\mathbf{C}_n^{1-\gamma_0}$ contains every cycle of $\mathbf{C}_n^{1-\gamma}$ and as well as some other cycles from $\mathbf{C}_n$) such that

$$\Pr\left(\left|\rho_{kk}(t) - \rho_{kk}^{1-\gamma_0}(t)\right| < \varepsilon e^{ct}\right) = 1, \tag{14}$$

where $\rho_{kk}^{1-\gamma_0}(t)$ is the perturbative expansion in (7) but calculated only with Feynman diagrams with cycles in $\mathbf{C}_n^{1-\gamma_0}$. Pr is a probability, and ε is a small positive number. Equation (14) says that the deviation of the approximated dynamics $\rho_{kk}^{1-\gamma_0}(t)$ of any individual electron in the ensemble is within εe^{ct} of the true dynamics $\rho_{kk}(t)$. A formal statement of these results and a proof are provided in the Appendix. Note that it does not appear to be possible avoid to the factor e^{ct} without introducing significant technical difficulties into the mathematics. The following analysis must be restricted to short times only. For real organic crystals in which c is expected to be in the order of $0.01\ \mathrm{fs}^{-1}$, we obtain an upper-bound error $\gamma e^{ct}/(1-\gamma)$ of 2.7% for $t = 100$ fs and of 7.4% for $t = 200$ fs when we set $\gamma = 0.01$. The approximations in Eqs. (13) and (14) are therefore relevant to the early stages of the electron interaction with the intermolecular vibrations of the lattice, which occur on a time-scale of at least 100 fs.[1]

In order to verify if the approximations in Eqs. (13) and (14) hold for the STB model, we must identify a set $\mathbf{C}_n^{1-\gamma}$ of correlated cycles that satisfy (12). A reasonable candidate for $\mathbf{C}_n^{1-\gamma}$ is cycles which are highly localised about site 0 in the lattice. The localisation of a cycle can be measured with the *cycle variance*. For a given cycle C containing vertices $v_1, v_2, \ldots, v_m$,[31] the variance of C is defined as

$$s_C^2 = \frac{1}{m}\sum_{k=1}^{m}(v_k - \bar{v}_C)^2, \tag{15}$$

where $\bar{v}_C$ is the *cycle mean*, $\bar{v}_C = (1/m)\sum_{k=1}^{m} v_k$. The cycle variance is shown for various cycles in Figure 4. A small variance means that the cycle is relatively localised across the lattice. Figure 5 shows a calculation of the cycle variance for all cycles with orders $n = 10, 12$, and 14 (the method used for generating the cycles is outlined in the Appendix). Figure 5 is interpreted as follows. Consider a set of cycles,

$$\mathbf{C}_n^q = \{C \in \mathbf{C}_n : s^2(C) > q\}. \tag{16}$$

(This notation is read as "the subset of cycles in $\mathbf{C}_n$ with variance greater than q.") The x-axis of Figure 5 is in units of q, and the y-axis of is the contribution of the cycles in $\mathbf{C}_n^q$ to the sum of degeneracies of $\mathbf{C}_n$. The plots show long tails and identify cycles with s_C^2 greater than about 1.5 as making a negligible contribution to the sum of the degeneracies. We expect similar results for cycles with lengths greater than 14; however, we were unable to perform this calculation due to hardware limitations. This analysis strongly suggests that we can identify the "important cycles," $\mathbf{C}_n^{1-\gamma}$ in Eq. (12) as the cycles with small variance, i.e.,

$$\mathbf{C}_n^{1-\gamma} = \{C \in \mathbf{C}_n : s_C^2 \le q\}, \tag{17}$$

where q is in the order of about 1.5 and γ is in the order of about 0.01. In order to visualise how many cycles from

FIG. 4. Degeneracies and variances of some cycles.

$\alpha(C) = 576$ $s^2 = 0.82$ $\alpha(C) = 3808$ $s^2 = 0.49$ $\alpha(C) = 21840$ $s^2 = 0.25$

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計することを目指す。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、多くの候補分子で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計、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!

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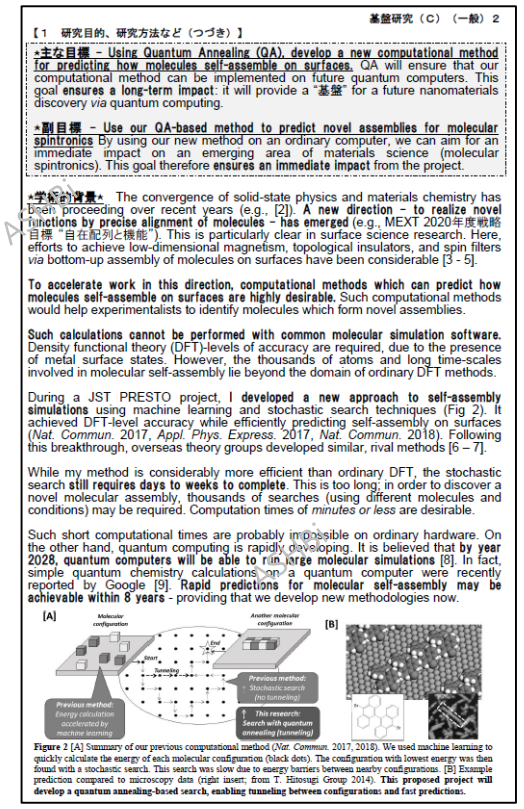
Figure 1. [A] Simple image of the molecular self-assembly process. [B] Project overview. I will write an algorithm for fast prediction of molecular self-assembly on a quantum computer. This will enable rapid computational screening for functional assemblies for nanotechnology applications.



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.

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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].

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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 insert; from T. Hitosugi Group 2014). **This proposed project will develop a quantum annealing-based search, enabling tunneling between configurations and fast predictions.**

Paper: Present a new result to specialists

Result is supported by analysis and formalism.
Effort required to read it.

Significance and impact are secondary.

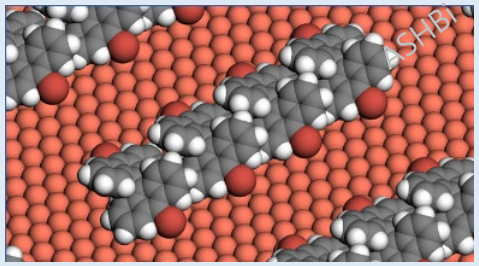
Proposal: Sell an idea

Idea is sold through rhetoric and visuals.
Little effort required to read it.

Significance and impact are paramount

Tip # 3: Clarify where your idea comes from

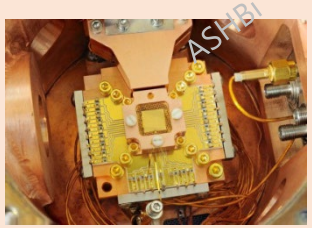
Past research



Simulation of nanomaterial assembly

Next step

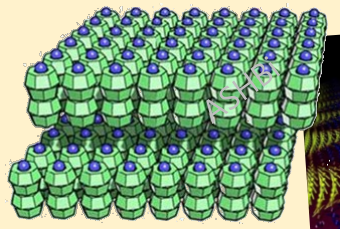
Project idea

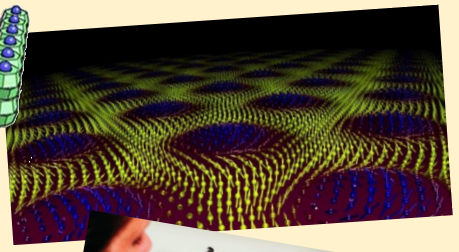


Simulation using a quantum computer

Previous step

Future vision





Design nanomaterials with ultrafast simulations

- Your idea should come from **two sources**: your past research and your future vision.
- Unlike a paper, your proposal must be grounded in **both the past and the future.**
- The past determines which steps you can take next. The future determines which of those steps has highest impact.

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-.
Research objectives, research method, etc. should be described within 4 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 originality, and creativity of the research project, (3) the circumstances leading to conception of the present research proposal, domestic and overseas trends related to the proposed research and the positioning of this research in the relevant field, (4) what will be elucidated, and to what extent and how will it be pursued during the research period, and (5) preparation status towards achievement of the purpose of the research project.

[SUMMARY]

"…the circumstances leading to conception of the present research proposal…"

Image sources: https://en.wikipedia.org/wiki/Self-assembly; https://algoanalytics.com/quantumAnnealers.html; 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/

My Kakenhi tips!

Before you write

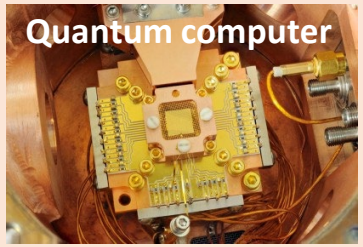
When you write

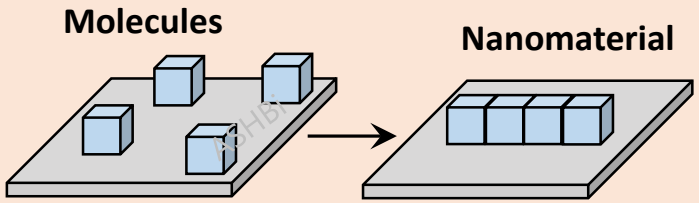
Tip # 4: On the first page, articulate your overall vision and sell it

Overall vision

Past research → *Next step* → ***Project idea*** ← *Previous step* ← ***Future vision***

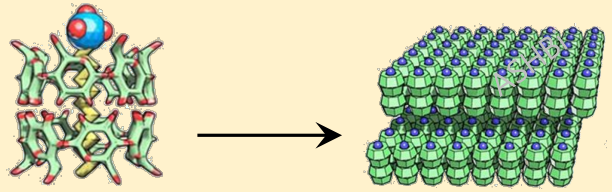
Project idea (step towards the big dream)





Simulate nanomaterial assembly using a quantum computer

Big dream

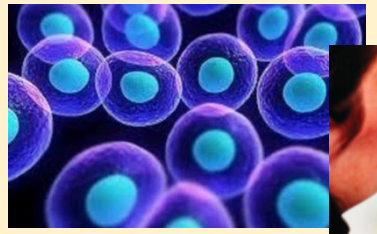


Molecule → **Nanomaterial**

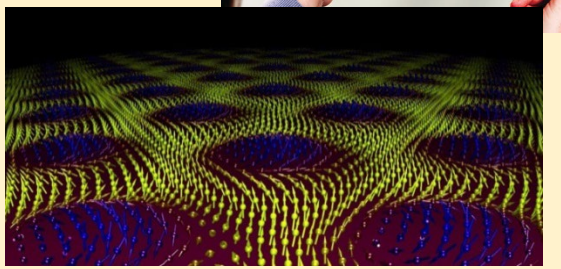
Simulate nanomaterial assembly *within seconds* (impossible with ordinary computers)

Big impacts

Artificial cells



Printed electronics



Ultrahigh density memory

Image sources:
https://en.wikipedia.org/wiki/Self-assembly
https://algoanalytics.com/quantumAnnealers.html
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/6563445/

Application form (first page)

Large scope

Specific focus

Large scope

Big dream

Impacts

Obstacle to big dream

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で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.

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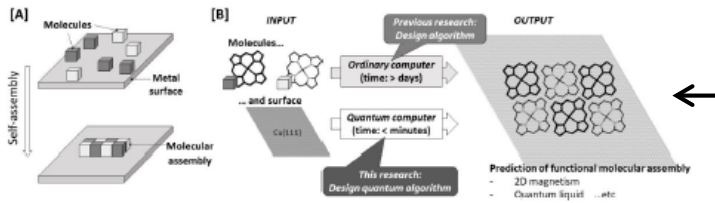

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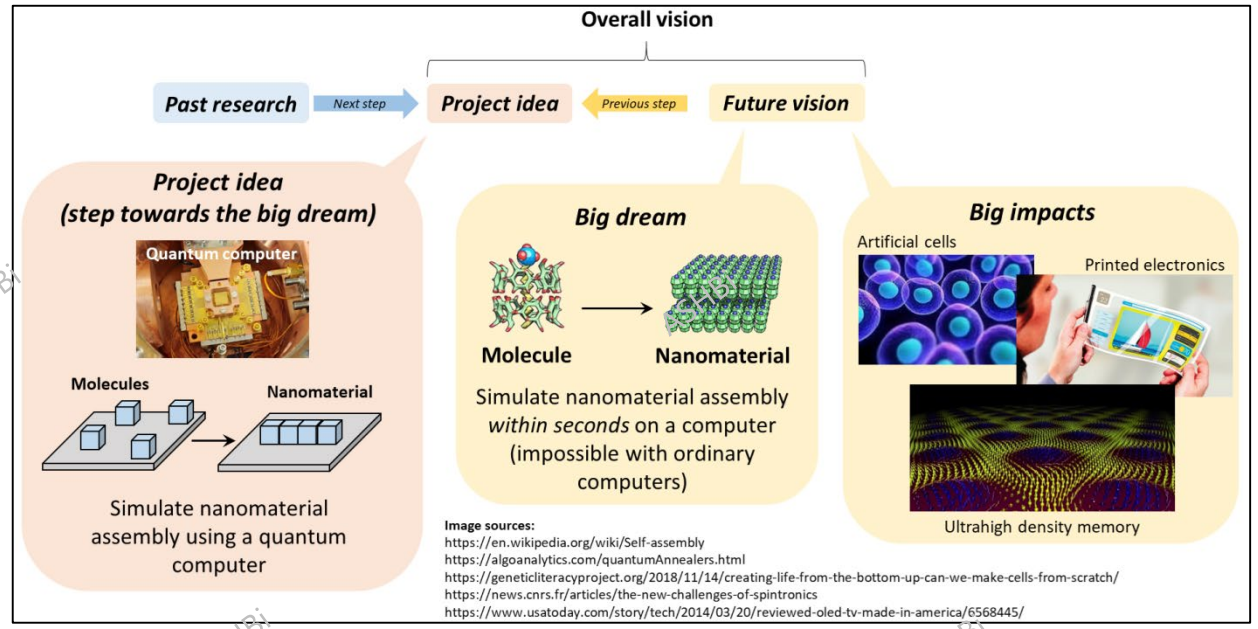

This project + impacts

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

基盤研究（C）（一般）1

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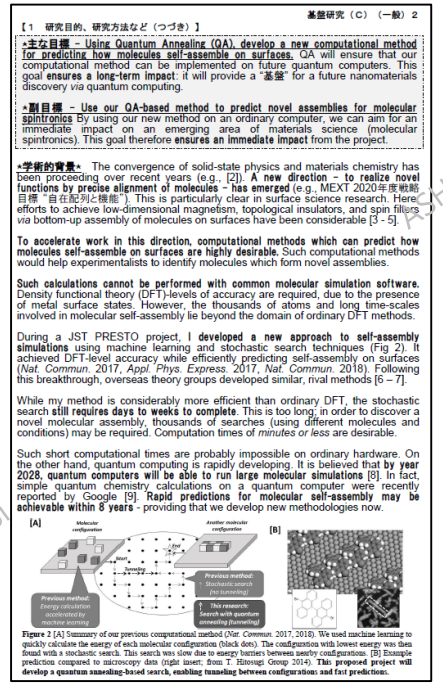
Fig 1. Summary of project



基盤研究（C）（一般）2

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Fig 2. Background / how this project overcomes previous bottlenecks

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

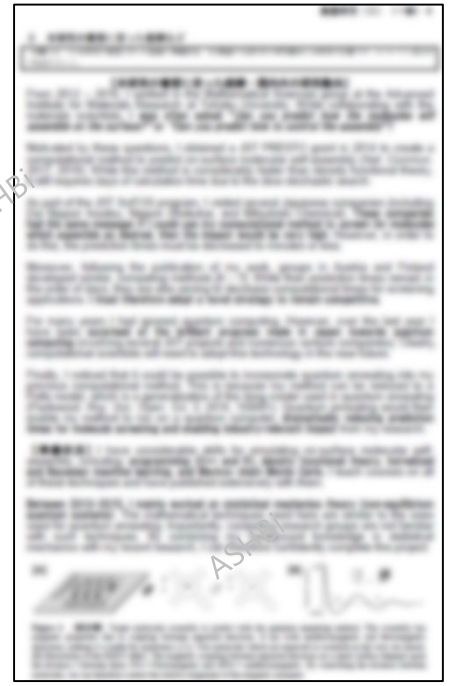
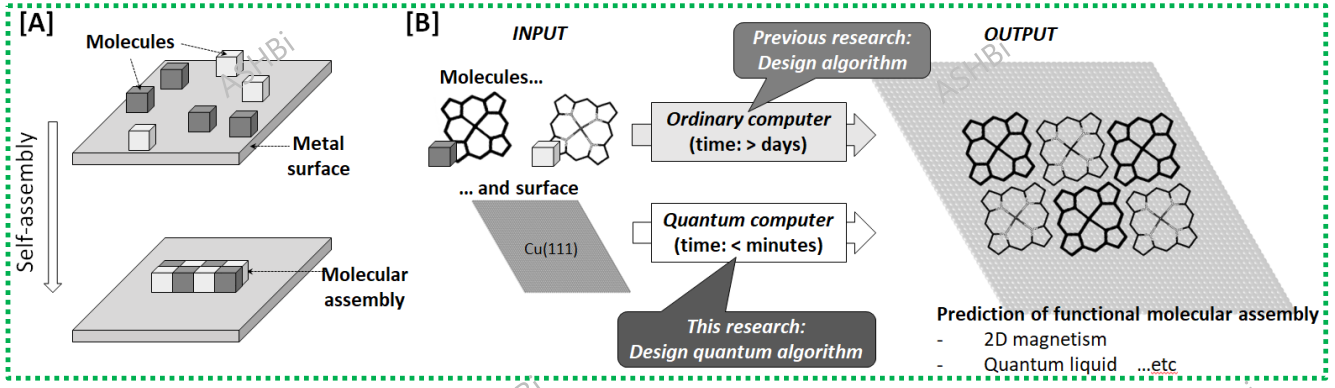


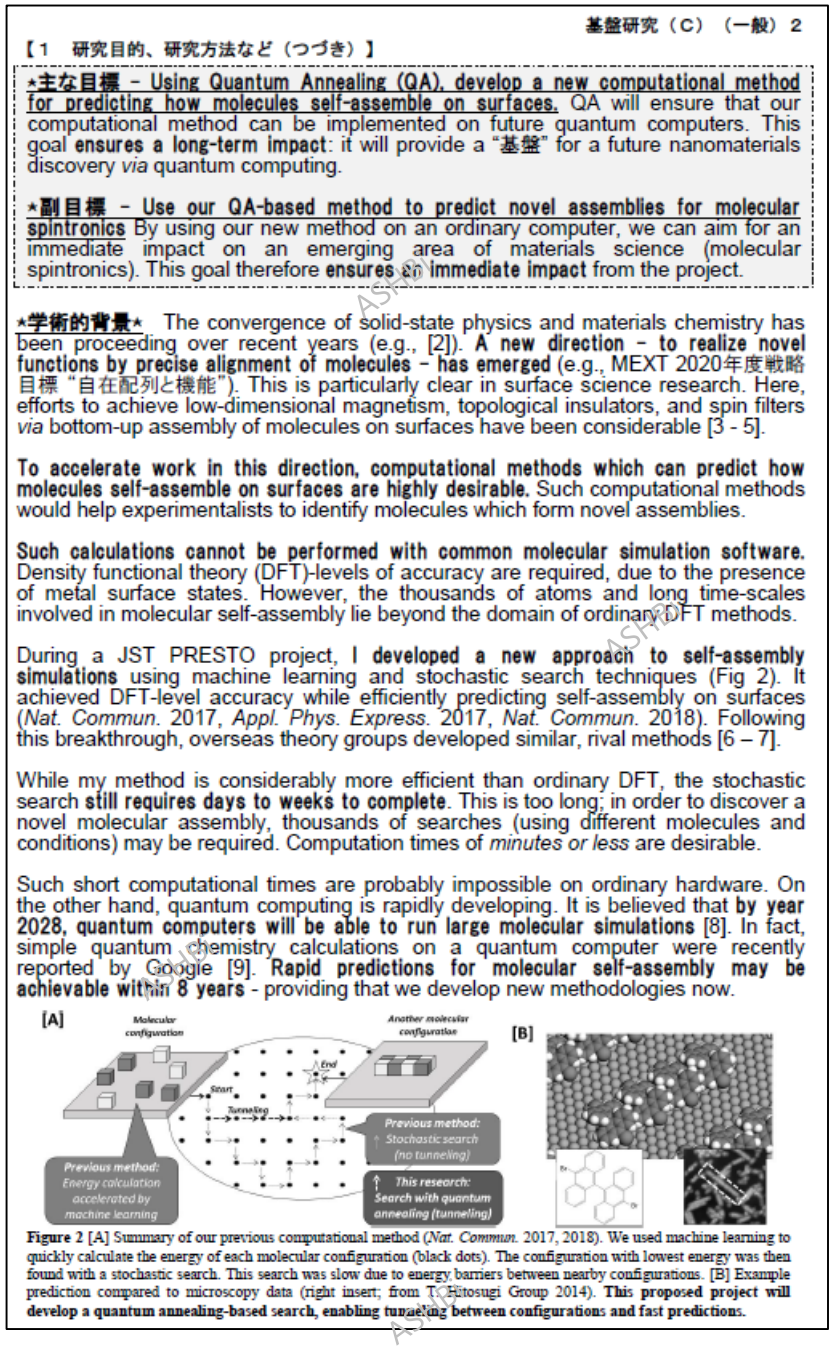
Fig 5 [because extra space was available] How to ensure immediate impact



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!



基盤研究（C）（一般）2

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⋆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 "自在配列と機能"). 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 insert; from T. Hitosugi Group 2014). **This proposed project will develop a quantum annealing-based search, enabling tunneling between configurations and fast predictions.**

Tip # 6: 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 # 7: Plan to spend most of your time editing

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

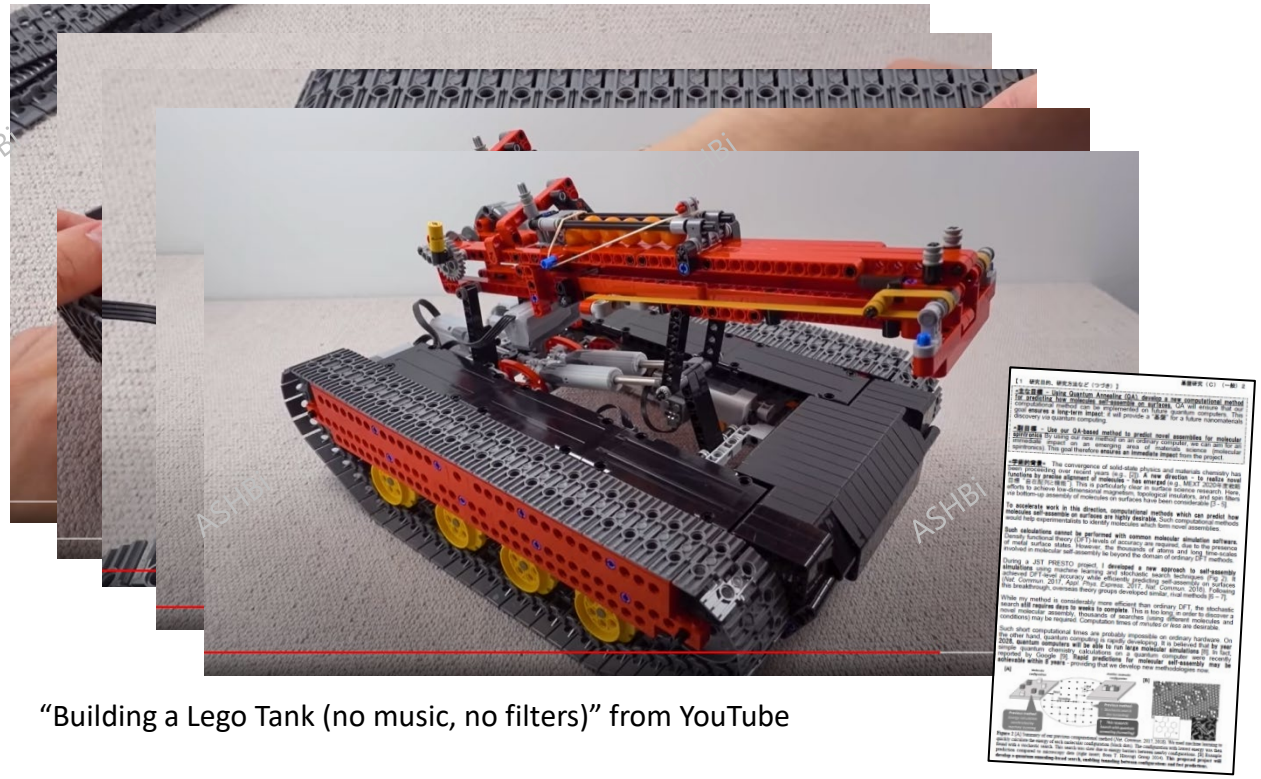
The convergence of solid-state physics and materials chemistry has been preceding over recent years. A new direction – to realise novel functionality by precise alignment of molecules – has emerged.

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 # 8: 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!

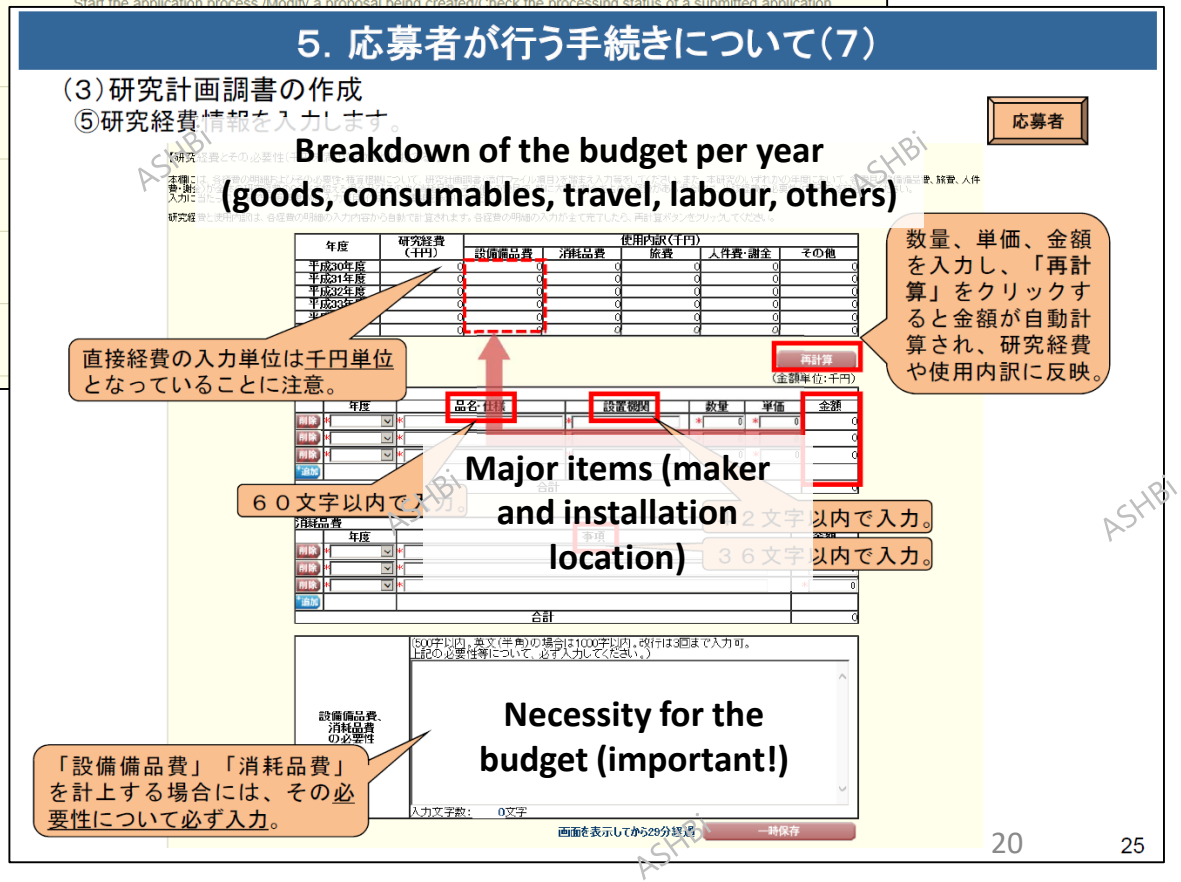
List of fields:
https://www.jsps.go.jp/english/e-grants/data/2020/09/R2b_kouboyoryo_e.pdf

Tip # 9: Familiarise 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

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

https://www.mext.go.jp/content/1395971_02.pdf



- As well as uploading your proposal, you must enter additional information (breakdown of money required and reasons).

My Kakenhi tips!

Before you write

When you write

But what about Japanese vs English?

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

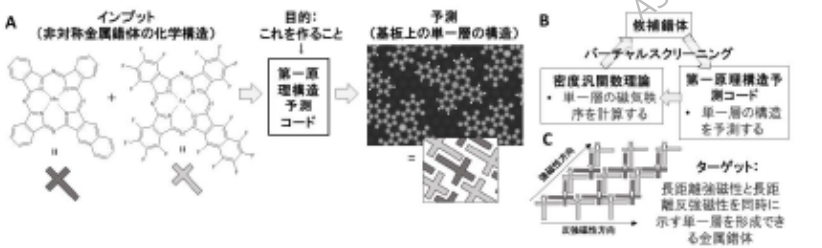


図 1. 本研究の目的・計画　(A)H31 年度は、非対称金属錯体の自己組織化で形成する単一層を対象とし、単一層の原子構造を予測できるコード(以下、FPSP コード)の開発を目指す。(B)H31 年度は、コードと密度汎関数理論によってバーチャルスクリーニングを行い、長距離磁気秩序を示す単一層を形成できる金属錯体の探索を目指す。(C)金属錯体の非対称性が引き起こす長距離磁気秩序の例。

（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。

Japanese vs English?

[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-translated text will leave a terrible impression – be careful

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.