【Nano tech 2024 Special Symposium】

How MI has changed Nanomaterials Development –Current Issues and Future Prospects–

Applications and Challenges in Computational Materials Development using Atomistic Simulator Matlantis

Preferred Computational Chemistry
Senior Manager Akihiro Nagoya

・2024 2/1 Thu. 15:00-15:40
・Main Theater[East hall 4]

self-introduction

Akihiro Nagoya
Preferred Computational Chemistry (PFCC)
Senior Manager, Technical Sales & Customer Success Department

Profile

- Completed Master's program, Graduate School of Engineering Science, Osaka University (2007)
- Toyota Central R&D Labs.
  - First-principles calculations: solar cell materials, semiconductor materials, fuel cell catalysts, graphene materials
  - Classical MD and MI of polymers
- ENEOS Corporation (2022)
  - Matlantis related services
- Preferred Computational Chemistry (2023)

Agenda

- About us
- Matlantis™: High-speed universal atomistic simulator
- User Case Study
  - Matlantis for Elucidation of Complex Phenomena and Screening of Materials (Dr. Onodera, ENEOS)
- Challenges and Perspectives
  1. useability
  2. overseas
  3. Difference in scale from experiment
- Summary

PreFerred Computational Chemistry (PFCC)

About Us

Company Name

Preferred Computational Chemistry

Established

June 1st, 2021

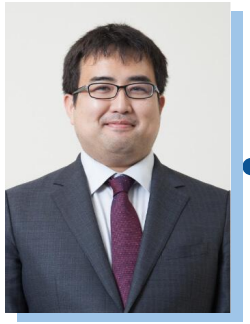
Preferred Networks

Japan's AI technology leader.

ENEOS

The largest petroleum company.

基本情報



Representative

Dr. Daisuke Okanohara

(CEO)

*July 2023 *rated 9.4/10 by IDTechEX*

- **Mission**

"*To accelerate materials discovery for a sustainable future.*"

- **Product: Matlantis™**: High-speed universal atomistic simulator

Matlantis™: High-speed universal atomistic simulator

Challenges in Materials Science

1

“To accelerate materials discovery for a sustainable future. ”

10^{60} of unknown molecules in the chemical space.

2

- ***Experiment*** used to be the mainstream but has faced throughput limitation.
- ***Computational Simulation*** *(e.g., DFT)* is often too computationally costly to be used in practical situations.
- ***Materials Informatics*** is a promising data-driven approach; however, “Universality” has always been challenging.

3

Simulation × Deep Learning

MATLANTIS

Materials Informatics

Mr. Shibata gave a talk at NanoTech 2023 (Speaker Deck)

日本一やさしい
マテリアルズ・インフォマティクスへの導き

～ 材料開発者は、マテリアルズ・インフォマティクスに何を求めるのか ～

PFCC　柴田ラビ

※ nano tech2023講演資料のうち、公開可能な部分のみ公開しております

1

https://speakerdeck.com/matlantis/ri-ben-yasasii-materiaruzuinhuomateikusuhenodao-ki-chai-tian-nanotech2023

Background

Materials Informatics (MI)

- The technology to accelerate the discovery and development of new materials using AI.
- Avoid the conventional trial-and-error approach without relying on the intuition or experience of researchers.

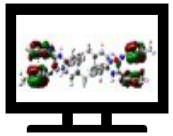
Conventional

Experiment

~10 times/month

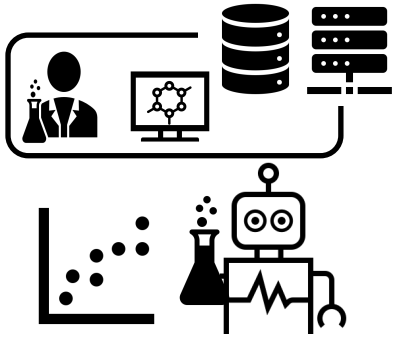
simulator

~10 times/month



MI

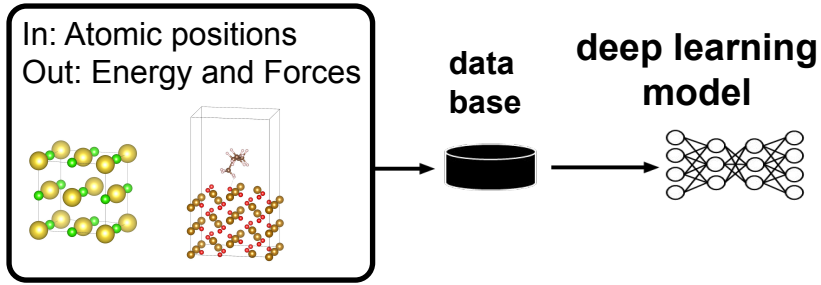
Experiments and calculations → Virtual experiments



Thousands of times/month

Matlantis

Calculations → Virtual experiments → Experiment



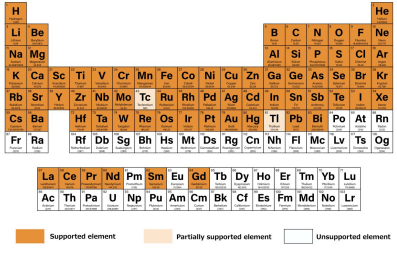
Universal simulator for predicting material properties from atomic configurations

製品の特長

2,000 years

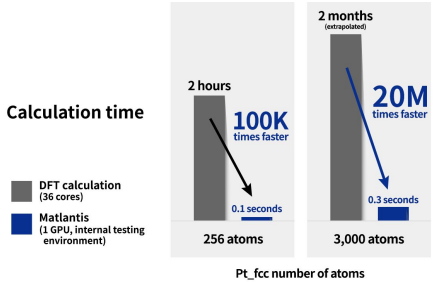
2,000 GPU years have been spent collecting DFT data sets.

72 elements

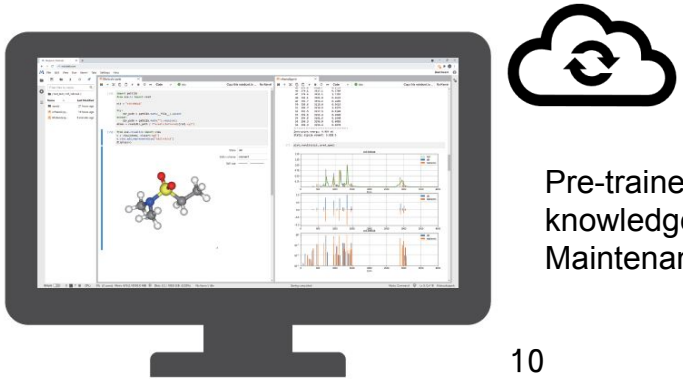


Applicable to **72 elements** and more.

20M times



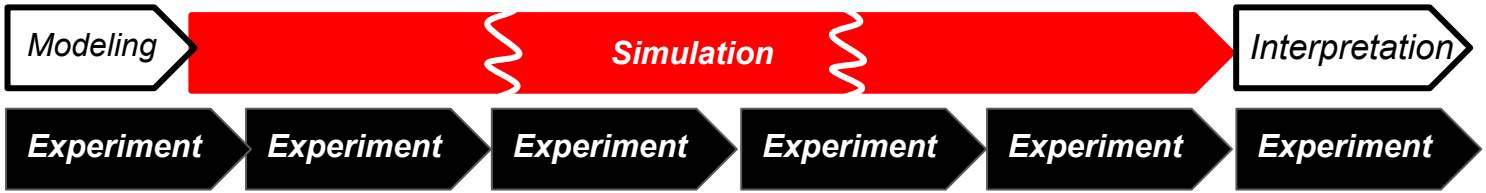
Up to **20M times faster** than typical DFT simulation.



Pre-trained AI model: no training data preparation or AI knowledge required
Maintenance free: No system/hardware specialist required

Why Matlantis™?

DFT Calculation



- Too long calculation time.
- Simplified simulation model and condition.
- Experiment followed by/parallel to simulation.

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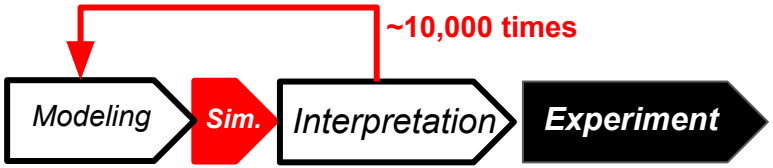
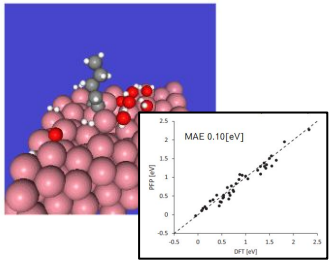


- Blazingly faster than DFT.
- Large-scale model, long physical time.
- Simulation-driven approach; iterative trial & error prior to experiment.
- **Dramatically accelerate the material development process.**

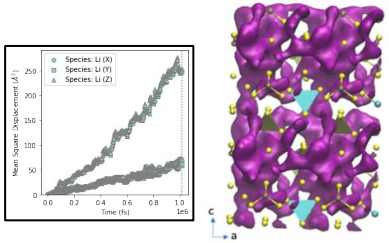
Applications

Catalyst



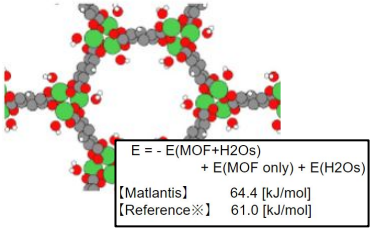
Large scale screening for optimal dopant species

Battery



Li diffusion in solid electrolyte

Adsorbent

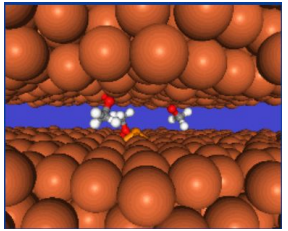


E = - E(MOF+H2Os)
+ E(MOF only) + E(H2Os)

【Matlantis】 64.4 [kJ/mol]
【Reference※】 61.0 [kJ/mol]

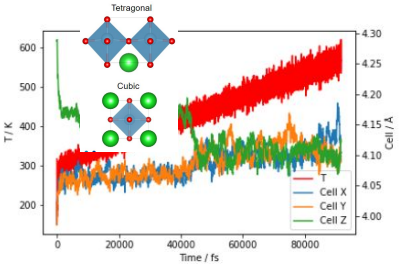
Adsorption energy in MOF

Lubricant



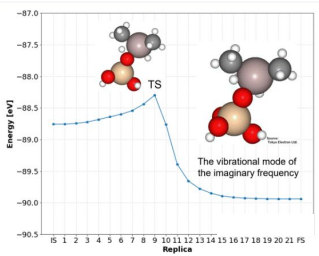
Tribochemical reaction

Ceramics



Phase transition in BaTiO3

Semiconductor



Reaction analysis of trimethylaluminum

Magnetic Materials

Separation Membrane

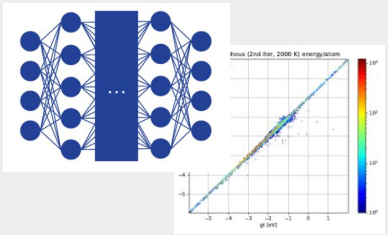
Metal&Alloy

⋮

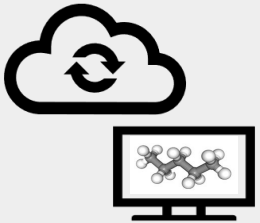
MATLANTIS

Our Services

Core Technologies



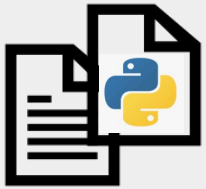
Universal Neural Network Potential



Cloud Computing Resources

Usability

Jupyter Lab Environment

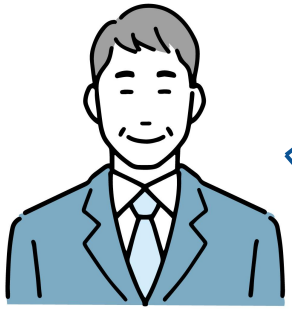


Documents and Sample Programs

Customer Support

Matlantis™ ユーザーの声：Toyota Motor Corporation

What took three months in
one week



10 million structures
per year.

Highly flexible and easy to apply.
Half of users
are from experiment team

https://www.youtube.com/watch?v=vMwIlr9v1x4

−Paradigm shift−
in materials development

Breakthroughs
+ in new materials

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Research Transformation by Matlantis™

https://www.slideshare.net/Matlantis/matlantis30-rula05ce05o175xpfcc20221215

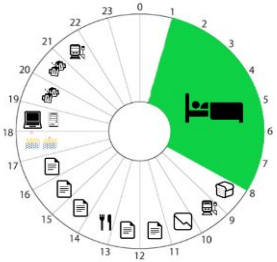
Previously

Comment from Prof. M. Koyama (Shinsyu Univ) during the press releases.

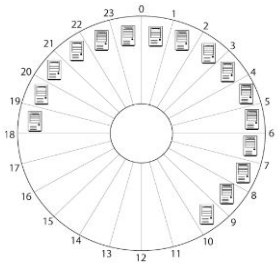
“ I've been looking at various methods for almost 20 years, but this is by far the most versatile I've touched. There is nothing but excitement.”

https://pc.watch.impress.co.jp/docs/news/1336421.html

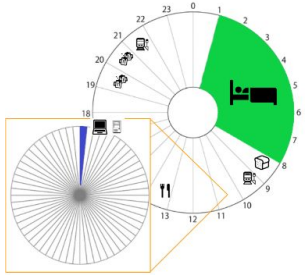
Researcher’s time



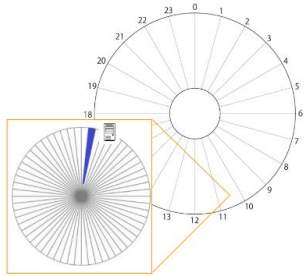
Computer’s time



Researcher’s time



Computer’s time



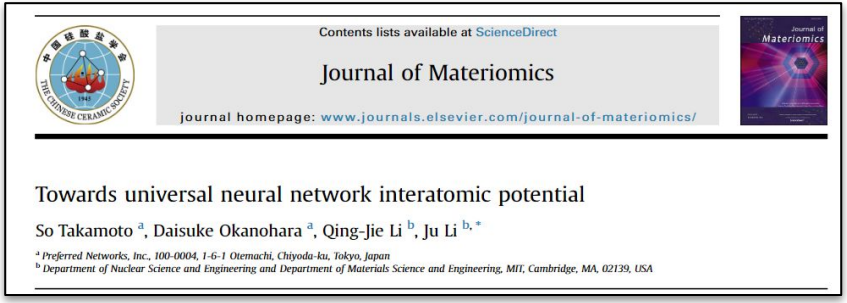
- Learn their intuition from experimental scientists
- Read papers carefully first

- Maintain computer in free time

- Run the calculations and show them to experimental scientists
- To read the paper carefully…
  - Create calculation models for a day/week + automate job submission
  - Automatically analyze the calculation results for a day/week.
- No need to maintain the computer

Scientific Papers

https://matlantis.com/cases



Contents lists available at ScienceDirect

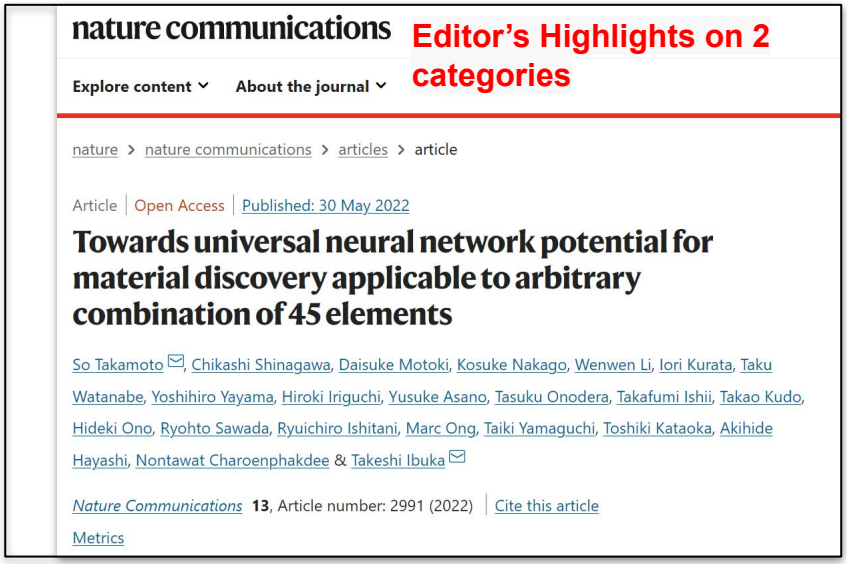
Journal of Materiomics

journal homepage: www.journals.elsevier.com/journal-of-materiomics/

Towards universal neural network interatomic potential

So Takamoto [a], Daisuke Okanohara [a], Qing-Jie Li [b], Ju Li [b, *]

[a] Preferred Networks, Inc., 100-0004, 1-6-1 Otemachi, Chiyoda-ku, Tokyo, Japan
[b] Department of Nuclear Science and Engineering and Department of Materials Science and Engineering, MIT, Cambridge, MA, 02139, USA



nature communications

Editor's Highlights on 2 categories

Explore content | About the journal

nature > nature communications > articles > article

Article | Open Access | Published: 30 May 2022

Towards universal neural network potential for material discovery applicable to arbitrary combination of 45 elements

So Takamoto, Chikashi Shinagawa, Daisuke Motoki, Kosuke Nakago, Wenwen Li, Iori Kurata, Taku Watanabe, Yoshihiro Yayama, Hiroki Iriguchi, Yusuke Asano, Tasuku Onodera, Takafumi Ishii, Takao Kudo, Hideki Ono, Ryohto Sawada, Ryuichiro Ishitani, Marc Ong, Taiki Yamaguchi, Toshiki Kataoka, Akihide Hayashi, Nontawat Charoenphakdee & Takeshi Ibuka

Nature Communications **13**, Article number: 2991 (2022) | Cite this article

Metrics

Other publications (as of July 2023):

Lieven Bekaert, et al.	2023	ChemSusChem2023, e202300676
Ayako TAMURA, et al.	2023	J. Comput. Chem. Jpn., 21, 129-133
Kan Hatakeyama, et al.	2023	10.26434/chemrxiv-2023-f9lxl
Tien Quang Nguyen, et al.	2023	J. Comput. Chem. Jpn., 21, 111–117
Lieven Bekaert,et al.	2023	J. Phys. Chem. C, 18, 8503–8514
Hiroshi Sampei,et al.	2023	JACS Au, 3, 991–996
Yuji Shitara,et al.	2023	Tribologist, 68, 280-291
Yuji Shitara and Shigeyuki Mori	2022	Tribologist, 67, 662-671
Tasuku Onodera	2022	Tribologist, 67, 821-829
Kaoru Hisama,et al.	2022	Comp. Mat. Sci., 218, 111955
So Takamoto, et al.	2022	Nature Comm.,13, 2991

+ 37 conference presentations

Customer Calculation Examples

Case Study: Material Screening with Matlantis

The 3rd Matlantis User Conference
Excerpts from materials provided by Dr. Onodera at ENEOS corporation

ENEOS

第3回 Matlantis User Conference

2023/07/21

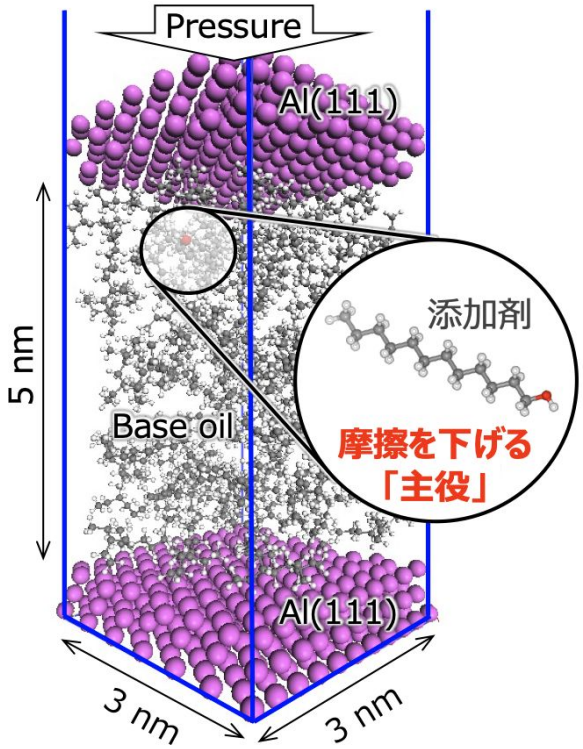
Matlantisによる複雑現象解明と材料スクリーニング ～潤滑油設計への応用～

小野寺 拓

ENEOS株式会社 中央技術研究所 デジタル研究所 MI技術グループ

ENEOS Corporation
[E'-ne-ohs]

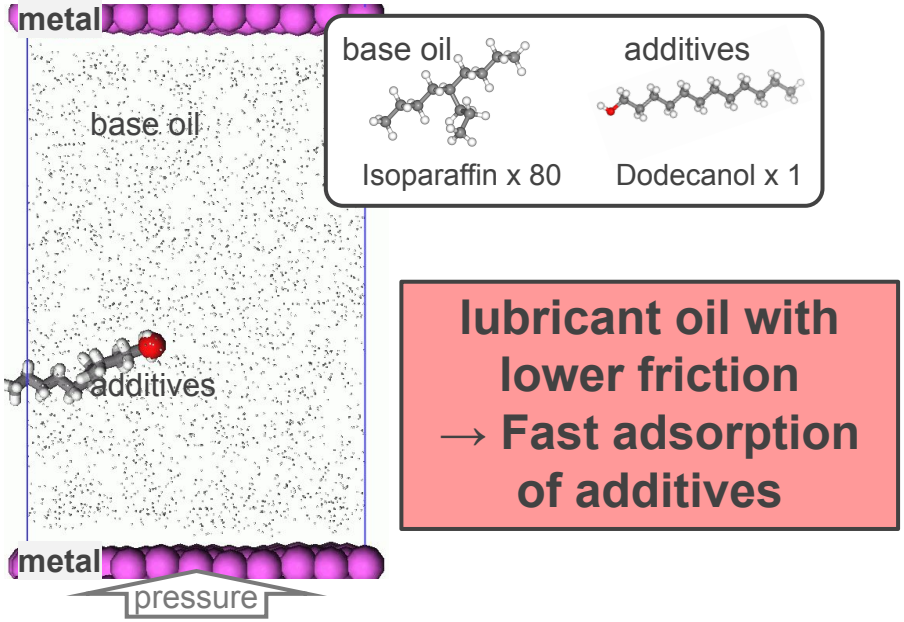
ENEOS Group Japan's Premier Energy and Materials Corporate Group



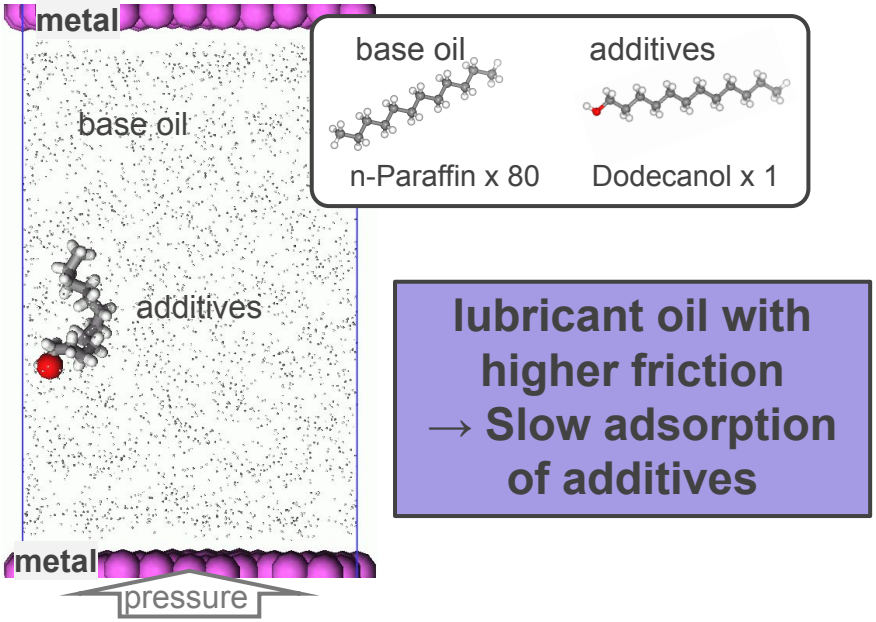
MATLANTIS

Lubricant additives for improved processability

Experimental results: **processability** varies with the type of base oil
⇒ Diffusion and adsorption dynamics of additives in two different base oils



lubricant oil with lower friction → Fast adsorption of additives



lubricant oil with higher friction → Slow adsorption of additives

Onodera, Tribologist, 67 (2022) 821 / Yamagishi et al, Tribology Conference 2022 Spring, Tokyo, D25 / Shibata et al, Tribology Conference 2022 Fall, Fukui, A23

How to find better lubricant oils?

Insights from MD simulations with Matlantis :

To reduce frictions, use a base oil
which forms a sparse oil film to facilitate additive adsorption

"design guideline"!

Machine learning based screening using simulation data representing the sparsity of base oil molecules

Proposal of base oil with low friction

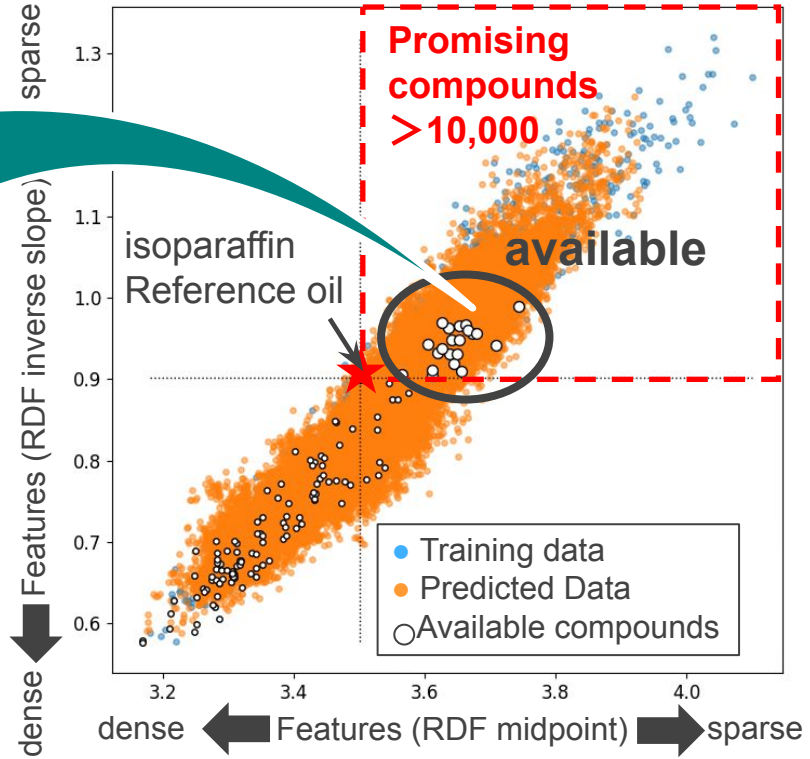
Three candidate compounds that are commercially available.
Experimental verification phase!

commercially available compounds

RDF feature	base oil for processing A	B	C	Reference oil
middle point	**3.74**	**3.70**	**3.68**	3.50
inverse slope	**0.99**	**0.94**	**0.96**	0.90

Promising candidate base oils for improved processability

(sparse oil film, fast additive adsorption)



ENEOS Corporation

Challenges and Prospects

Issue 1: Usability

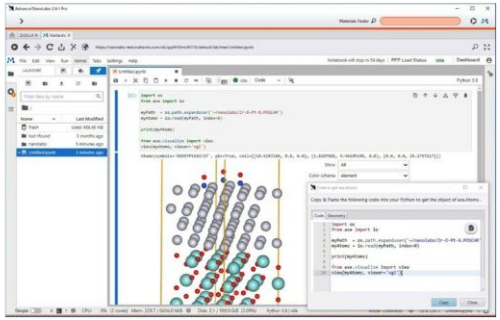
Cloud services via a browser are difficult to automate.

Python programming is difficult. I want an intuitive GUI.

I need immediate support by phone.

I can't do it myself, so I want to outsource the simulation.

Functional Integration between “Advance/NanoLabo“ and "Matlantis"



(Advance/NanoLabo に搭載された Matlantis 連携画面)

Training programs with SkillUpNext

MATLANTIS

Learning Materials and Customer Support

Atomistic Simulation Tutorial

- Document: https://docs.matlantis.com/atomistic-simulation-tutorial/en/
- Code: https://github.com/matlantis-pfcc/atomistic-simulation-tutorial

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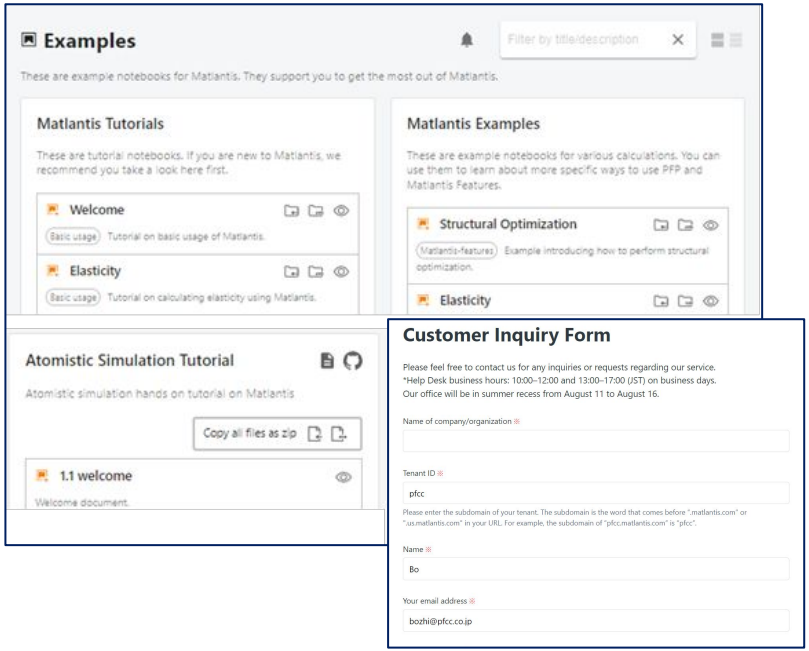
Expert customer support

- Inquiry form
- support meetings
- Sample programs



ChatGPT

反応のしやすさを調べるシミュレーションの方法を教えて

反応のしやすさを調べるシミュレーションとしては、化学反応の遷移状態理論（Transition State Theory）や反応速度論を用いた計算化学の手法が一般的です。ここでは、化学反応のしやすさを計算するための基本的な手順を紹介します。

1. **量子化学計算**:
   まず、反応に関与する分子の電子構造を量子化学計算により求めます。これには密度汎関数理論（Density Functional Theory, DFT）やハートリー・フォック法（Hartree-Fock method）などが用いられます。
2. **最適化と遷移状態の探索**:
   反応物と生成物のエネルギー最小構造を最適化します。次に、反応物から生成物に変化する過程でのエネルギーが最高点になる遷移状態（活性化エネルギーのピーク）を探索します。これには、saddle pointの探索や、反応座標の推定に基づく方法などがあります。
3. **振動解析**:
   遷移状態および安定な反応物・生成物の振動解析を行い、エネルギーの最小かつ二次の極大点（遷移状態）を確認します。遷移状態では一つの虚数振動モードが存在します。
4. **エネルギーバリアの決定**:
   反応物から遷移状態へのエネルギーバリアを計算し、このエネルギーバリアが反応のしやすさを決定します。
5. **Eyring方程式やArrhenius方程式の適用**:
   手に入れたエネルギーバリアを使い、Eyring方程式やArrhenius方程式に基づく反応速度定数

ASEを使って遷移状態を求めるpythonプログラムを書いて

ASE（Atomic Simulation Environment）は、Pythonで書かれたパッケージであり、様々な原子スケールのシミュレーションタスクを行うことができます。遷移状態を求めるには、エネルギー最適化と遷移状態を探索するアルゴリズム（いわゆるsaddle pointを見つけるアルゴリズム）が必要です。

以下は、ASEを使用して遷移状態を探索する基本的なPythonプログラムの概要です。ここでは、ASEでサポートされている計算エンジン（以下の例では`calc`として表される）を使用しており、実際の計算には適切なエンジンを選択し、設定する必要があります。

python　　Copy code

```python
from ase import Atoms
from ase.optimize import BFGS
from ase.calculators.emt import EMT
from ase.constraints import FixAtoms
from ase.neb import NEB
from ase.io import read, write

# 例としての反応物と生成物の構造を定義
reactant = read('reactant.traj')
product = read('product.traj')

# 遷移状態探索のためにNEB(nudged elastic band)オブジェクトを作成
number_of_intermediate_states = 5
```

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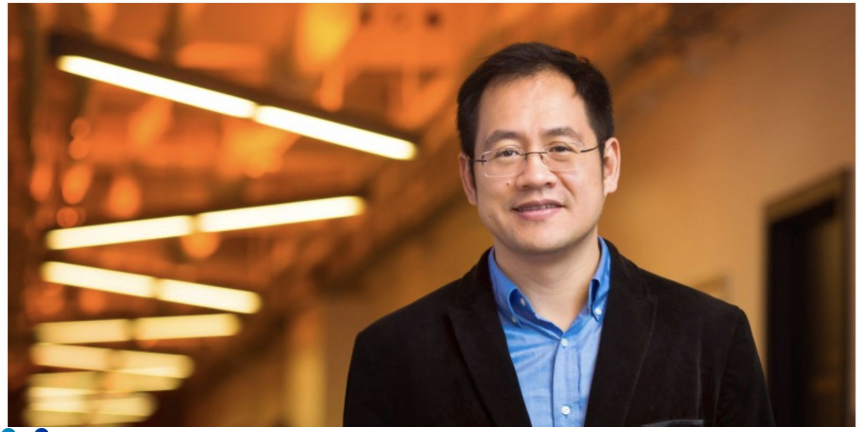
Issue 2: Overseas Expansion

2023.04.18 Event

Free Webinar with MIT Professor Ju Li: Invention and Applications of Universal Machine Learning Interatomic Potential

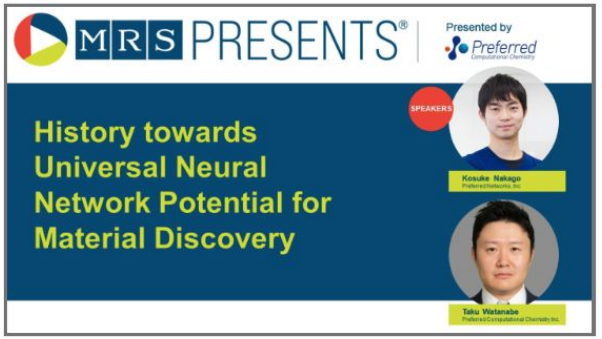
USA: Monday, May 29, 2023 at 7:00 – 8:30 pm ET | 4:00 – 5:30 pm PT
Japan: Tuesday, May 30 at 8 – 9:30 am JST
Zoom Webinar
Presented by: Ju Li, Professor at Massachusetts Institute of Technology

Matlantis™ will host a free webinar presented by Ju Li, a professor at the Department of Nuclear Science and Engineering and Department of Materials Science and Engineering at Massachusetts Institute of Technology (MIT), titled *The Invention and Applications of Universal Machine Learning Interatomic Potential.* The webinar will be held via Zoom at 7 – 8:30 pm Eastern Time (USA) on Friday, May 26, 2023. Registration will be free.



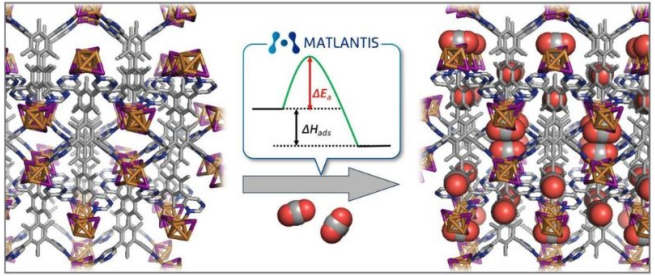
2023.09.19 Event

Webinar Appearance at MRS: History towards Universal Neural Network Potential for Material Discovery



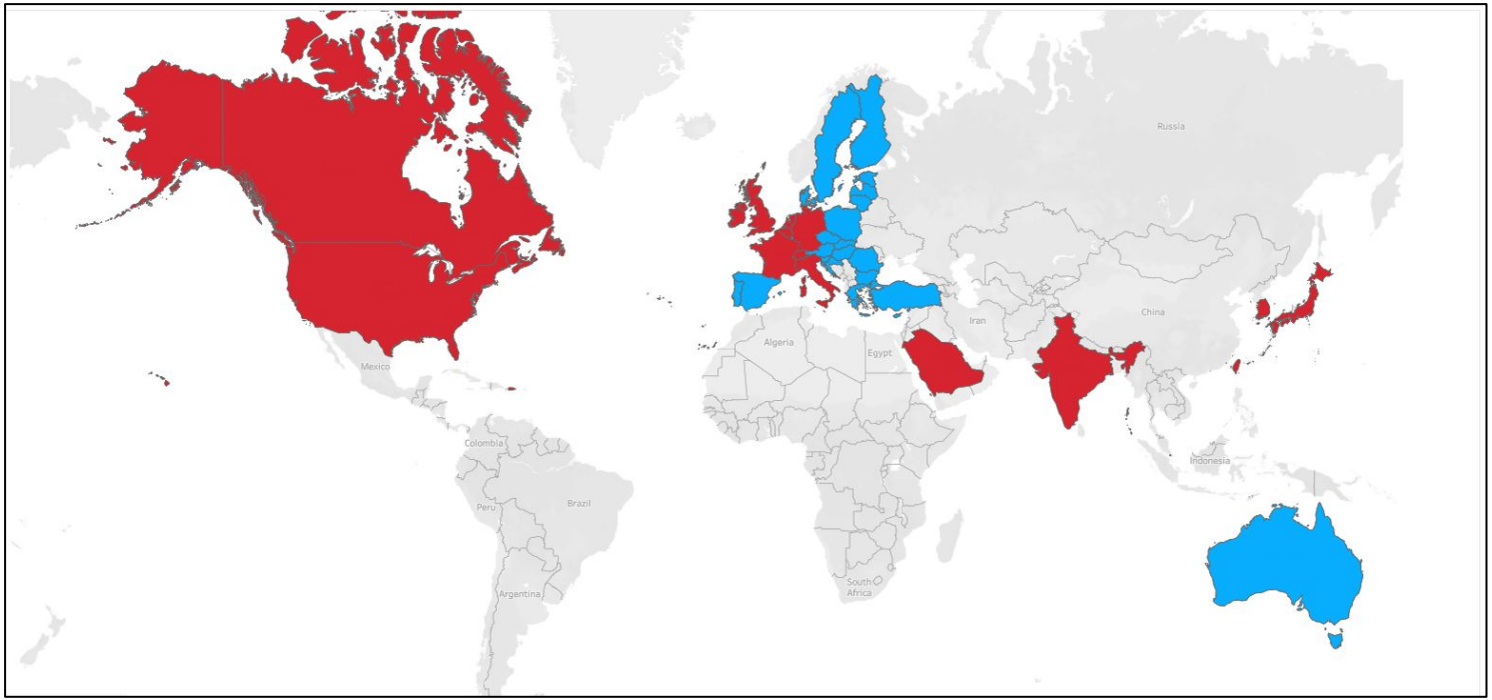
2023.10.13 Event

Webinar on Nov. 22 with the Royal Society of Chemistry: CO_2 storage, magic doors, and machine learning.

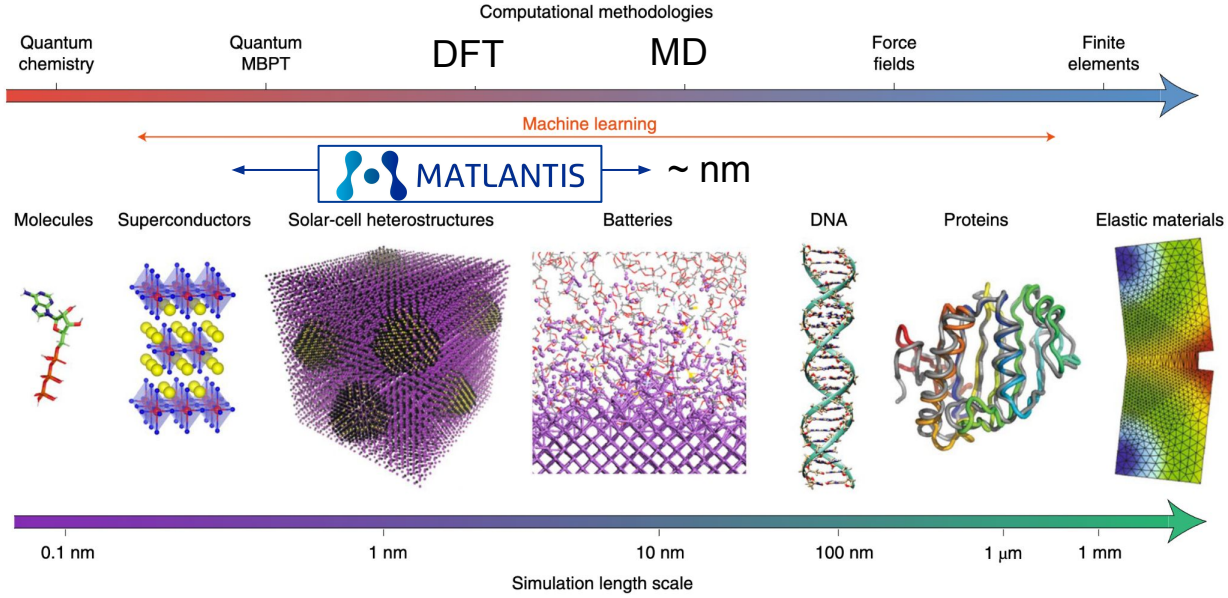


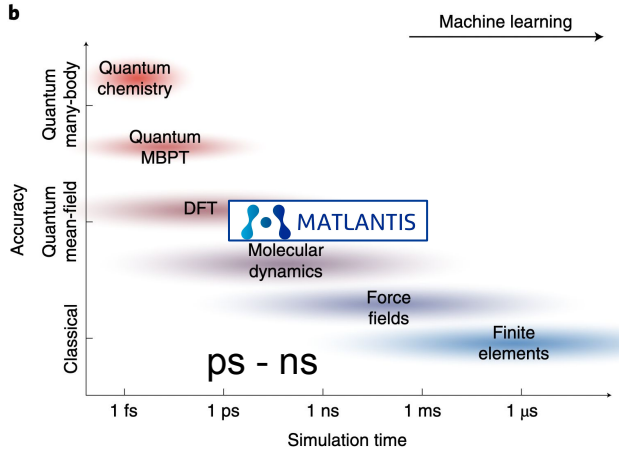
User base of Matlantis

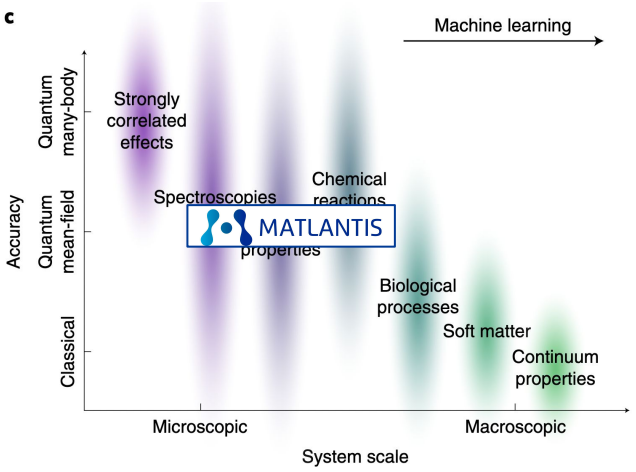
- Available Countries and Regions. (As of January 2024)



Issue 3: Difficulties in Scale







S. G. Louie, Nature Materials, 20, 728 (2021)

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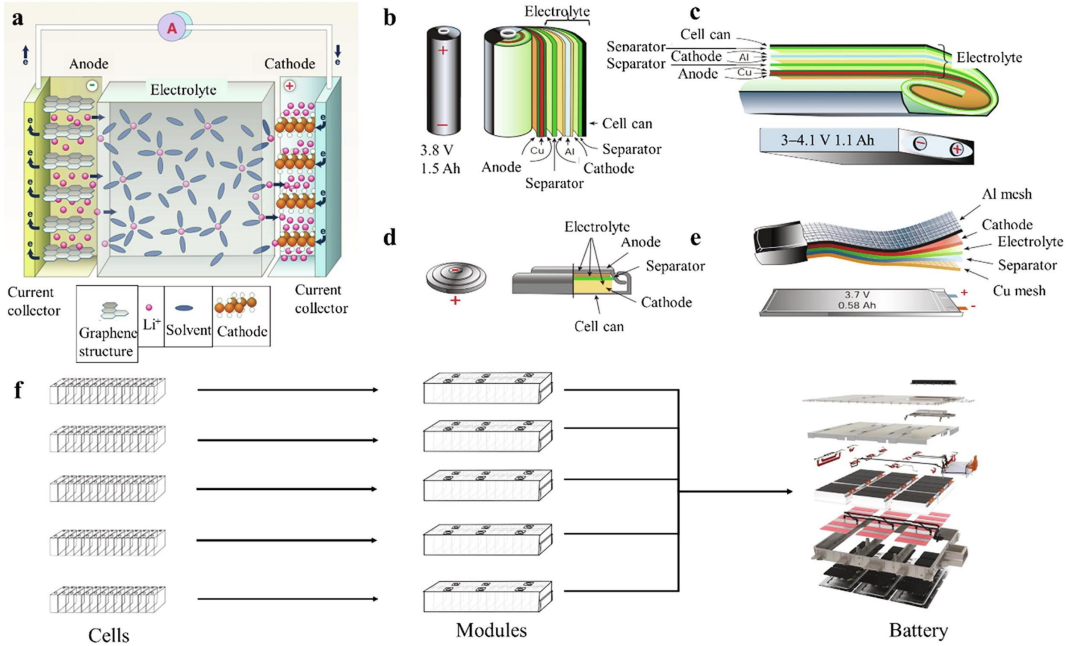
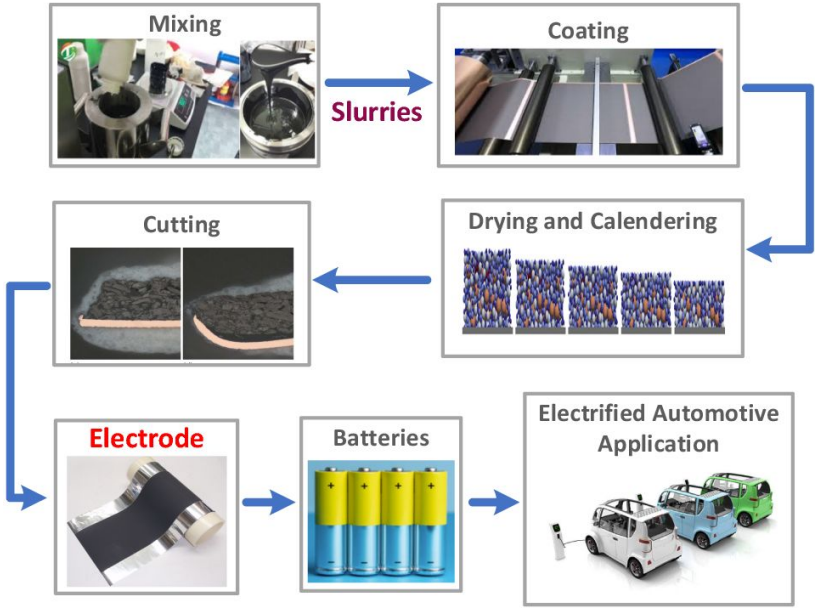
Difficulties in Scale: Device Structure of Li-ion Batteries

Materials, Cells, Modules



Y. Chen, Journal of Energy Chemistry 59, 2021, 83-99

Experiments



K. Liu, Automotive Innovation, 5, 2022,121

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summary

- **Matlantis™** can dramatically accelerate material discovery and mechanism elucidation of your interest.
- **Matlantis-driven approach** will enable you to perform large scale screening for materials discovery in a realistic time scale.
- **Matlantis™** will facilitate the DX of your R&D department.


Preferred
Computational Chemistry