EIG CONCERT-Japan　国際共同研究「原子レベルでの材料設計」 2023 年度　年次報告書	
研究課題名（和文）	グリーン H_2 生産のための原子層状ヘテロ構造の機械学習主導のボトムアップ設計
研究課題名（英文）	Machine-learning-driven bottom-up design of atomically-layered heterostructures for green H_2 production
日本側研究代表者氏名	Dr Mohammad Hussein Naseef AL ASSADI Prof Paolo MELE Prof Sarp KAYA; Dr Esmaeil DOUST KHAH HERAGH Dr José Julio GUTIERREZ MORENO
所属・役職	RIKEN Center for Emergent Matter Science (JAPAN), Researcher Shibaura Institute of Technology (JAPAN), Professor Koç University (Türkiye), Professor; Koç University (Türkiye), Researcher Barcelona Supercomputer Center (Spain) Researcher
研究期間	2023 年 4 月 1 日　～　2026 年 3 月 31 日

1．日本側の研究実施体制

氏名	所属機関・部局・役職	役割
Dr Mohammad Hussein Naseef AL ASSADI	創発物性科学研究センター, Research Scientist	Principal Investigator (PI)
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2．日本側研究チームの研究目標及び計画概要

この提案は，電気および光触媒による H_2 製造用の原子制御されたヘテロ構造薄膜を理解、設計、および合成することを目的としています。提案されたワークフローは次の通りです。

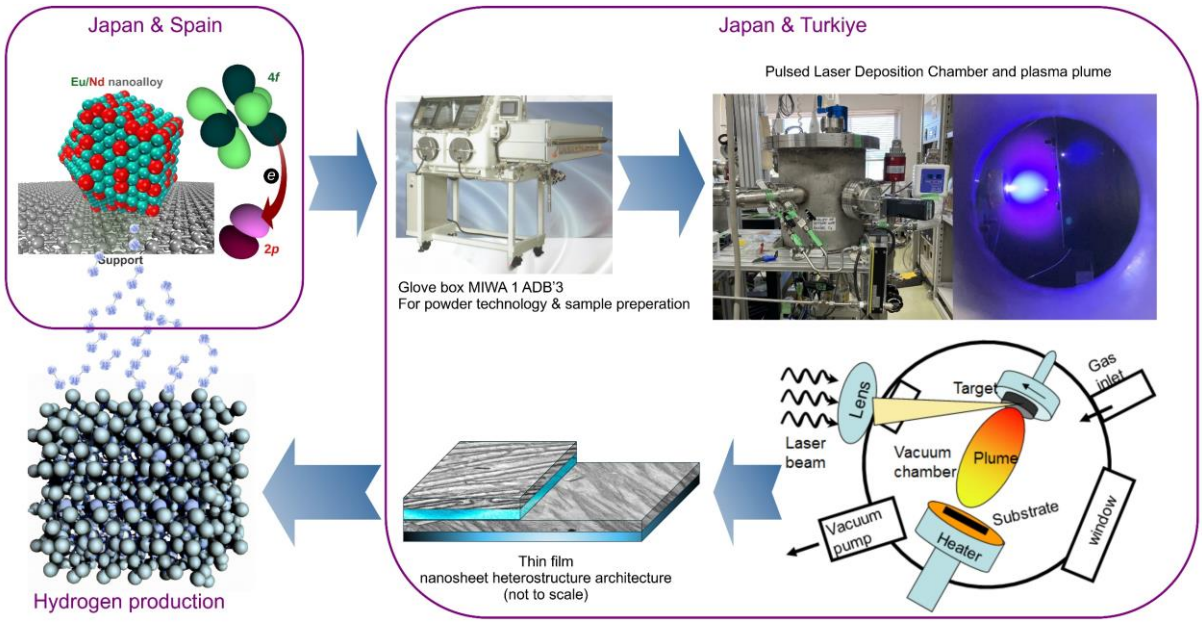
1.トレーニングセットを作成するための高スループット密度汎関数計算

2.機械学習を使用して、検索ドメインを数百万のヘテロ構造に拡張する
3.原子制御された薄膜技術を使用した優れた予測の合成と特性評価

この提案は、量子化学と機械学習に基づく最先端の理論的ガイダンスと、パルスレーザーおよび原子層蒸着を用いたサンプルの制御された合成をめざします。この方法で目標とする合成されたサンプル品質は、原子レベルでの制御のない従来の手法を用いた場合の組成、サイズ、界面などが根本的に不均一であるものと比べて、圧倒的に高品質なものが実現できます。

3. 日本側研究チームの実施概要

Public Release



Our research team is excited to share significant progress in developing cost-effective catalysts for hydrogen production based on metallic nanoalloys. Focused on metallic nanosheets with a palladium (Pd) structure, we conducted high-precision calculations for around 70 compounds, exploring two surface terminations and 11 dopants at three concentrations. Palladium is renowned for its efficiency in catalysing hydrogen production from formic acid, but its high cost necessitates innovative solutions to make it more affordable. Our simulations aimed to identify chemical trends that enhance catalytic activity through various doping modifications.

These extensive simulations were carried out using high-performance computing facilities at the Barcelona Supercomputer Centre (Spain) and RIKEN, employing the open-access software package SIESTA. Our team dedicated considerable effort to optimising numerical settings and rigorously verifying the accuracy of the pseudopotentials, setting the stage for more efficient calculations in the future.

Preliminary findings from these simulations have already informed experimental work on Pd/Ag and pure Pd thin films at Istinye University (Turkey), highlighting the practical impact of our theoretical studies. This integration of theory and experiment is crucial for advancing the development of economically viable catalysts for

hydrogen production.

Furthermore, we are enhancing our research capabilities with new equipment at the Shibaura Institute of Technology, ensuring we maintain cutting-edge facilities. The installation of an advanced glove box will support the fabrication of nanosheet metallic and ceramic heterostructures, furthering our work on this project.

Our collaborative efforts have also yielded promising results with Pt-based nanoflakes on porous carbon nitride and Pd nanoparticles on functionalised silicate surfaces. These findings have led to one journal publication and two conference proceedings, with additional manuscripts under review:

1. E. Doustkhah, A. Kotb, T. Balkan, M. H. N. Assadi “Metal–Support Interaction in Pt nanodisk–Carbon Nitride Catalyst: Insight from Theory and Experiment” (2024) *Nanomaterials* 14(11), 921; https://doi.org/10.3390/nano14110921
2. S S Kabir, M H N Assadi “Detrimental 2*p*–3*d* Hybridisation in Ni Nanosheets Supported on Strontium Dioxide for Catalytic H_2 Production, Necessitating Thickness Optimisation” *Energy Proceedings* 44 (2024). https://doi.org/10.46855/energy-proceedings-11059
3. M H N Assadi “Critical Dimensionality Effects in Europium Nanosheets Supported on Titanium Dioxide for Catalytic Hydrogen Production” *Energy Proceedings*, Accepted, (2024).

Looking ahead, we are thrilled to announce the “3rd International Nanotech-Eurasia Conference” to be hosted by Istinye University in Turkey (Sept 5-7, 2024) and a symposium on “Innovations in Energy Materials” at the TMS Annual Meeting in Las Vegas (March 23-27, 2025). These events will provide platforms to share our latest discoveries and foster further advancements in this vital field.

The Spanish team at the Barcelona Supercomputer Center helped with the complex computer calculations. They provided the software, set it up efficiently, and wrote programs to analyse large amounts of data generated by hundreds of density functional calculations automatically. The Turkish at Istinye University (Istanbul) team designed the experimental set-up based on the current theoretical results. Subsequently, they synthesised nanoparticles with platinum and palladium using the atomic layer deposition technique. These samples have shown good catalytic activity and were then sent to Japan for further analysis at RIKEN and the Shibaura Institute of Technology.