NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE | Graduate College

Joint PhD Program Description

The description for the Joint PhD program will be posted online as a sub-page to Joint/Dual PhD Programmes | Graduate College | NTU Singapore.

Name of Partner University	Sorbonne Université
City, Country	Paris, France
Year of Establishment	2015
Program	☒ Joint Degree ☐ Joint Supervision
Description of the Program (150-250 words)	Established in 2015, the NTU-Sorbonne joint PhD degree program is providing students with a unique opportunity to explore a thesis project in an interdisciplinary and intercultural environment. Students in the program will have two thesis advisors – one in NTU, Singapore and one in Sorbonne, Paris – and will have to fulfil a residency of 12 months at the Partner University. Upon completion of the degree requirements, the students will be awarded doctorate degrees jointly by NTU and Sorbonne. Candidates interested in any of the joint projects are advised to contact either the Sorbonne or NTU supervisors for additional information on the project as well as admission requirements.
Disciplines	• Natural sciences (physics, chemistry, materials science, energy) • Modelling and engineering • Life sciences, health and medicine • Social sciences • Humanities • Business and management
PMC Names and Emails	NTU: • Sierin Lim (SLim@ntu.edu.sg) • Leong Weng Kee (chmlwk@ntu.edu.sg) Sorbonne: • Souhir Boujday (souhir.boujday@sorbonne-universite.fr) • Bertrand Granado (bertrand.granado@sorbonneuniversite.fr)

NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE | Graduate College

Joint Projects

Home University	Nanyang Technological University	
Supervisors	**Home**	**Partner**
Name	Sierin Lim	Olivier Pluchery
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Website	https://www.ntu.edu.sg/cceb	Institut des NanoSciences de Paris
Project Title	**Understanding Charge Transport on Hybrid BioNanoparticles**	
Project Description (200-300 words)	Charge transport is found in nature under various forms such as electronic conduction, quantum tunnelling or ionic migration. These phenomena have strong connections and applications for organic/molecular electronics. While charge transport in inorganic nanostructures have been widely studied, explorations on the phenomena on hybrid bionanoparticles (hbNP) are scarce. hbNP provide an intermediate model for understanding the charge transport mechanisms, between the complexity of natural structures and the inorganic nanoparticles. Learning from nature will help replicating these principles into organic electronics. In this project, the student will: (1) design and synthesize hbNP made of various metals (e.g., gold) using ferritin (protein-based iron-storage molecule) as a template; (2) develop experimental approaches to study how electrical charges build up and shape the assemblies of HbNP using advanced techniques based on atomic force microscopy (AFM) such as Kelvin Probe Force Microscopy (KPFM); (3) formulate design principles for applications of bionanoparticles in organic electronics. Pre-requisites: practical knowledge on molecular biology and basic knowledge on nanoscience Beneficial prior knowledge/skills: operations of atomic force microscopy Skills to learn: hybrid nanoparticle synthesis, AFM, KPFM	
Program/Center Website(s)	N/A	
Additional Information (e.g., files with project details)	NA	

NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE | Graduate College

Joint Projects

Home University	Nanyang Technological University	
Supervisors	**Home**	**Partner**
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Project Title	**Understanding the Role of Transglycosylase in Bacterial Cell Wall Synthesis**	
Project Description (200-300 words)	Antibiotics resistance is an extremely serious problem in public healthcare, and the rapid spread of multidrug-resistant bacteria is becoming a pandemic of global proportions. On 1 November 2017, Singapore has launched national strategic action plan to support global call for action against antibiotics resistance. Peptidoglycan is the core component of all bacteria cell walls, and bacteria cell wall synthesis has become the primary target process for nearly all new antibiotics development. However, one of the key bottlenecks in developing antibiotics that target the bacteria cell wall synthesis process, has been the unavailability of peptidoglycan substrates, from either natural or synthetic sources, for mechanistic studies and novel antibiotics development. This program is to rationally design and synthesize functional peptidoglycan derivatives for diagnostic and therapeutic aims. We will investigate PG-based metabolic labelling of bacterial cell surface. We will also conduct structure-based drug design and transform transglycosylase (TGase) substrate into inhibitor by editing the structure of PG. With no doubt, this project is the platform that holds great promise for the development new generation of antimicrobial therapeutics and diagnostics. It will help Singapore to achieve the anti-infectious disease strategies and goals by building new capabilities and offering a differentiated value proposition.	
Program/Center Website(s)	NA	
Additional Information (e.g., files with project details)	NIL	

NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE | Graduate College

Joint Project Details

Home University	Nanyang Technological University	
Supervisors	**Home**	**Partner**
Name	Assoc. Prof. Lee Jong-Min	Dr Axel Wilson
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Project Title	**Electrocatalyst Design through Modulating Dual-Atomic Coordination on Monolayered Elemental Substrates**	
Project Description	Developing high-efficient electrocatalysts for water electrolysis and fuel cell applications is crucial to the pursuit of a sustainable energy future. Constructing electrocatalysts by rational design at the atomic level has been increasingly regarded as a promising approach thanks to recent advances in material characterization and theoretical comprehension. In particular, dual-atomic nanoarchitecture is gaining significant interest due to the enormous possibility of structure modulation toward realizing novel reaction mechanisms. In comparison to the state-of-the-art single-atom electrocatalyst, the presence of two active sites in close proximity enables strong synergism, leading to significantly enhanced catalytic performance. Furthermore, the controlled coordination of two atoms allows precise control over the reaction intermediates and reaction pathways, thereby improving the selectivity toward the desired products. Besides, the dual-atom configuration provides mutual support, preventing atom agglomeration or detachment during catalytic reactions and thus enhancing operational stability. Recently, various post-graphene 2D elemental materials have been developed, attracting substantial interest owing to the rich structural chemistry and enhanced anisotropic electron transport triggered by unique Fermi surface topography. More importantly, in contrast to carbon-based materials, the non-carbon elemental 2D materials feature strong interaction with metallic atoms, allowing electronic modulating and stabilizing of the dual-atom structures simultaneously. Herein, I hypothesized that the precise coordination modulating of dual-atomic moieties grown on monolayer elemental 2D materials will enable significantly enhanced catalytic performance. To explore the hypothesis, in this project, I will target three key objectives as follows • Devise a facile synthetic pathway to prepare dual atoms confined on monolayered elemental 2D substrates. • Characterize materials' chemistry, nanostructure, and electrocatalytic performances.	

	• Investigate the structure-function relationship using theoretical simulation and Operando studies. The developed electrocatalysts with high performance and excellent long-term stability would be further characterized in pilot scale for real-life applications. More importantly, this project will provide insightful guidance for the rational design of advanced electrocatalysts, facilitating the translation of scientific research to industrial applications.
Project Details	**a) Specific aims and expected outcome** The scientific and technological challenges targeted in this project are to design a superior electrocatalyst via confinements of dual-atom nano architectonics on monolayered elemental substrates and to explore the underlying structure-function relationship to optimize the material's performance toward electrochemical water splitting. Over the course of this project under NTU-Sorbonne joint supervision, three key objectives will be pursued: 1. Devise a facile synthetic pathway for the preparation of dual atoms confined on monolayered elemental 2D substrates 2. Characterize materials' chemistry, nanostructure, and electrocatalytic performances 3. Investigate the structure-function relationship through theoretical simulation and Operando studies The resulting electrocatalysts would possess novel nanostructures and precisely tailored surface microenvironments that favourably promote electrochemical water splitting, thereby enhancing energy efficiency. Furthermore, the electrocatalysts developed in this project would exhibit high performance and excellent long-term stability, enabling their evaluation in pilot-scale applications for real-life scenarios. Notably, the insights gained from this project will provide valuable guidance for the rational design of novel electrocatalysts, facilitating the translation of scientific research into practical industrial applications. **b) Significances** **Green hydrogen production from water electrolysis, powered by renewable electricity, promises an excellent pathway for sustainable energy transition**. Since proposed by John Bockris in the 1970s,[1] green hydrogen has been hailed as a revolutionary alternative to fossil fuel for a sustainable energy future. It offers several advantages, including superior gravimetric energy density and clean combustion products.[2, 3] For instance, pressurized gaseous and liquid hydrogen exhibit approximately three times higher energy density (approx. 142 MJ/kg) compared to gasoline, diesel, and liquefied natural gas.[4] This high energy density makes green hydrogen an attractive option for energy storage and transportation. Unlike grey and blue hydrogen produced through steam-methane reforming (SMR), green hydrogen is generated through water electrolysis powered by renewable electricity, resulting in zero emissions.[5] One of the key benefits of green hydrogen is its ability to effectively address the

intermittent supply of renewable energy. By converting renewable electricity into hydrogen chemical energy, it enables the storage and utilization of energy based on end-user demands. Furthermore, green hydrogen is highly versatile as it can be directly consumed in fuel cells or further processed to produce other electro-fuels such as e-methanol and decarbonized ammonia. This versatility supports the widespread deployment of renewable energy technologies. Nations like Japan are putting drastic efforts toward realizing a "hydrogen society", in which hydrogen is regarded as the major component of the nation's secondary energy framework.[6] National Renewable Energy Laboratory of the U.S. Department of Energy proposed a vision defined as H_2@Scale with hydrogen seamlessly incorporated into the overall energy system in an integrated or hybridized fashion for servicing all society's energy demands.[7] (**Figure 1**) Hydrogen Council's study ("Hydrogen scaling up") anticipated that by 2050, hydrogen could meet 18% of the world's final energy demands, create a market with revenues of 2.5 trillion dollars, provide 30 million jobs, and decarbonize sectors like transport, industry, and residential by between 40-60%.[8] In Singapore, hydrogen is identified as a critical component in the nation's efforts to achieve its net-zero emission target by 2050, as outlined in the Energy 2050 Committee report by Singapore's Energy Market Authority.[9] While significant momentum is growing for green hydrogen as its energy system-wide benefits become clear, substantial challenges remain for green hydrogen to achieve its full potentials: high production cost (($4.02-$6 vs $2 produced by SMR)[10, 11], low performance, and poor durability of water electrolysis systems.[12]

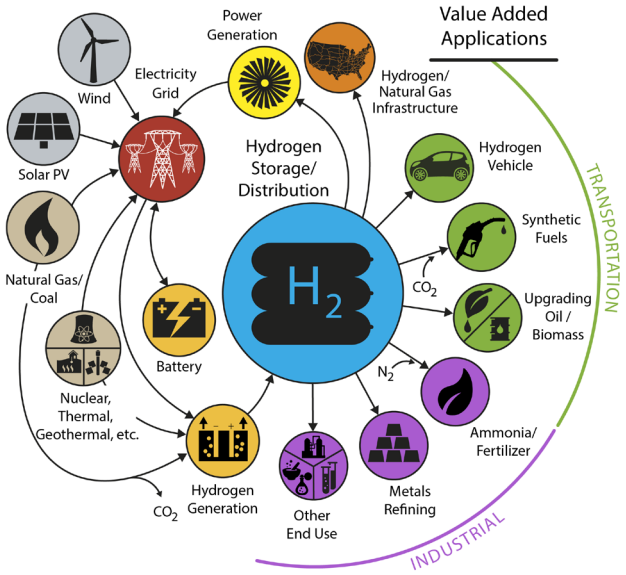

Figure 1. With efficient transformational technologies, Hydrogen can be seamlessly incorporated to our energy network, featuring different energy resources, and servicing all society's demands. Adapted from H_2@Scale initiative.

	Cost-efficient, highly active, and durable electrocatalyst for electrochemical green hydrogen technology is still lacking. Currently, considerable expense associated with water electrolysis technology stems from the cost of the electrocatalysts inevitably used to expedite the sluggish electrode reactions, namely the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). For instance, in Proton Exchange Membrane (PEM) electrolysers, the electrocatalysts account for a significant fraction (38%) of the total membrane cost,[13] highlighting the importance of improving their performance and cost efficiency. The state-of-the-art electrocatalysts for water electrolysis, such as Pt/C for HER and Ir/Ru-based oxides for OER, exhibit significant drawbacks.[14] One notable weakness is their low atomic utilization caused by large particle size, resulting in low mass activity and high production cost. Moreover, the electrocatalysts often suffer from structural deterioration, leading to unstable long-term performance (even up to 95% current drop observed in laboratory test [15]). Besides, these catalysts are solely active for a single electrochemical reaction (either HER or OER). Meanwhile, from the commercialization perspective, multifunctionality is highly desirable as it simplifies the structures of electrolyzer, reduces operational costs, and prevents cross-contamination issues. These disadvantages severely affect the viability of the wide-scale production of green hydrogen from water electrolysis. **Fabricating electrocatalysts through the precise construction of dual-atom nano-architectonics represents a new frontier in the next-generation electrocatalysts**. Dual-atom (DA) materials are gaining significant interest due to the enormous possibility of structure modulation toward realizing excellent catalytic performance.[16] As a mesophase between nanocluster (NC) and single-atom catalysts (SA), DA exhibits ultimate atomic utilization, superior to that of NCs, while also providing unparalleled tunability in both atomic and electronic configurations compared to SACs.[17] Notably, DA nano-architectonics takes advantage of the unique properties and synergistic effects that arise from the close proximity and specific coordination of two different atoms within a catalyst structure.[18] Besides, the dual-atom configuration provides mutual support, preventing atom agglomeration or detachment during catalytic reactions, thus enhancing the long-term stability of the catalyst.[19] The precise controlling of the spatial arrangement and electronic properties of these dual atoms enables the optimizations of catalytic activity, selectivity, and stability simultaneously for various electrochemical reactions. This level of control allows for fine-tuning of the catalyst's electronic structure, surface chemistry, and surface area, which are critical factors influencing catalytic activity. For example, Wang et al. modulated Fe-Fe dual atom nanostructure via the incorporation of S atoms. The resulting non-planar nest-like [Fe_2S_2] nano-architectonics exhibit superior activity toward electrochemical oxygen reduction, which is attributed to the favorable co-regulation of atomic composition and spatial configuration at the dual active sites.[20]

While dual-atom materials have shown great promise in electrocatalysis, their current development has predominantly focused on utilizing carbon-based substrates, which inherently exhibit severe disadvantages, most notably low conductivity, and is highly susceptible to corrosion at high applied potentials. The limitation of the C-based substrate greatly impedes the wide-scale application of dual-atom electrocatalysts. Recently, various post-graphene 2D elemental materials have been developed, attracting substantial interest owing to the rich structural chemistry and enhanced anisotropic electron transport triggered by unique Fermi surface topography.[21] More importantly, in contrast to carbon-based materials, the non-carbon elemental 2D materials feature strong interaction with metallic atoms, allowing electronic modulating and stabilizing of the dual-atom structures simultaneously. We postulate that the utilization of non-carbon elemental 2D materials would open up new possibilities for developing highly efficient and stable dual-atom electrocatalysts for high-performance electrochemical applications.

c) Approach and methodology

Devise a facile synthetic pathway for the preparation of dual atoms confined on monolayered elemental 2D substrates. During the first phase of this project, facile methods will be devised to synthesize dual-atom nanostructures incorporated into monolayered elemental 2D substrates. Appropriate elemental 2D substrates will be selected based on their properties, such as conductivity, stability, and compatibility with the target dual-atom catalyst. The selected 2D substrate will be then prepared via epitaxial growth on a salt template with precise controlling of reaction parameters to favour the formation of monolayered morphology. Subsequently, the dual-atom moiety will be incorporated onto the functionalized surface of the elemental 2D substrate utilizing various deposition techniques such as incipient wetness impregnation, solid-phase deposition, and electrodeposition, depending on the nature of the interaction between the dual-atom nano architectonic and the elemental substrates. Annealing reduction or thermal treatment will be applied to enhance the bonding and stability of the dual atoms on the substrate. This step can facilitate the formation of desired active sites and promote the interaction between the dual-atoms moiety and the substrate.

Characterize materials' chemistry, structure, and electrocatalytic performances. Materials morphology, nanostructure, chemistry, and compositions will be elaborately explored using various analysis techniques with a particular focus on interrogation of the dual atomic nanostructure, surface topography, and electron configuration. The results will be used to validate the feasibility of synthesis approaches and obtain insights into the formation mechanisms of the materials. Materials' electrocatalytic performance will be characterized using

	conventional potentiostat set-ups focusing on the structure-performance and activity-stability relationships. Specifically, scanning and transmission electron microscopies (SEM and TEM, respectively) will be employed to characterize the materials' morphology. Scanning Probe Microscopy (SPM) such as scanning tunnelling microscopy (STM) and atomic force microscopy (AFM), can provide high-resolution imaging of the surface topology. These techniques can reveal the arrangement and distribution of dual atoms on the substrate. The dispersion of dual atoms can also be observed by aberration-corrected TEM (ACTEM) operated in high-angle annular dark-field scanning transmission electron microscopy mode (HAADF-STEM). The sample compositions and elemental distribution will be probed using Energy dispersive X-ray spectroscopy (EDS). Importantly, the local atomic structure and electron configuration of the dual atom nano architectonics will be probed using X-ray absorption spectroscopy. The obtained X-ray absorption near edge structure (XANES) and Extended X-Ray Absorption Fine Structure (EXAFS) will be analysed to gain comprehensive insights into the atomic structure at the dual-atom centers. **Investigate the structure-function relationship through theoretical simulation and Operando studies.** Understanding of structure-function relationship is of critical importance in rational development of novel electrocatalysts. Density Functional Theory (DFT) calculations will be conducted to provide valuable insights into the electronic structure, bonding, and catalytic properties of dual-atom materials. By modelling the atomic arrangement and studying the energetics of reactant adsorption, reaction intermediates, and transition states, DFT can provide valuable insights into the reaction mechanism and energetics. Furthermore, Molecular Dynamics (MD) will be employed to study the dynamic nature of dual-atom materials and their interactions with the active species and electrolytes. These calculations will provide valuable information about the stability of the dual atoms under polarized electrocatalytic conditions. Theoretical simulations can help elucidate the reaction mechanisms occurring on dual-atom materials. By simulating various reaction pathways and considering different surface configurations, theoretical studies can provide insights into the intermediates, transition states, and rate-determining steps, thereby establishing the structure-function relationship. The reaction mechanism as well as the structural evolution of the dual-atom nano architectonics under operating condition will be further studied employing various Operando techniques. Operando X-ray Absorption Spectroscopy will be employed to monitor the changes in the electronic and structural properties of dual-atom materials during catalytic reactions, providing insights into the active site structures and reaction intermediates. Furthermore, Operando Raman and Infrared Spectroscopy can be employed to study the changes in structure of

	elemental 2D substrate under operating condition. Besides, Electrochemical operando techniques, such as electrochemical impedance spectroscopy and in-situ electrochemical scanning tunnelling microscopy (EC-STM), can also be employed to study the electrochemical behaviour and surface restructuring of dual-atom materials under working conditions. These techniques provide insights into the catalyst's stability, active sites, and reaction mechanisms during electrochemical reactions. By combining theoretical simulations and operando studies, a comprehensive understanding of the structure-function relationship of dual-atom materials can be obtained. Theoretical simulations provide insights into the material electron properties and reaction energy, while operando studies provide real-time information about the dynamic response of the catalyst under working conditions. The comprehensive insights obtained facilitate the optimization and design of dual-atom materials with enhanced catalytic performance for water electrolysis application. **d) Research plan** Over the course of this project under joint supervision, the synthesis of the electrocatalyst, preliminary material characterization and electrochemical characterization will be conducted under the supervision of Prof. Lee Jong-Min (NTU supervisor). Subsequently, the advanced materials characterization including ACTEM, STM, and ex-situ and in-situ X-ray absorption spectroscopy will be conducted under the supervision of Dr. Axel Wilson (Sorbonne Université). Finally, the DFM and MD simulation studies will be conducted under joint-supervision of both supervisors. **e) Supervisor Expertise** Prof. Lee Jong-Min is an associate professor in School of Chemistry, Chemical Engineering and Biotechnology (CCEB) and Energy Research Institute at Nanyang Technological University (NTU). Prof. Lee's research is highly interdisciplinary with immersive research experiences in electrochemistry, green chemistry, and nanotechnology. He has coordinated several research projects at NTU, and his works led to over 200 high-impact research articles published in leading journals, such as Nat. Energy, Nat. Commun, JACS, Angew. Chem, Adv. Mat, Adv. Ener. Mat. Dr. Axel Wilson is a researcher at Centre national de la recherche Scientifique-Sorbonne University. He has strong research expertise in field of physico-chemistry of functional surfaces, heterogeneous

	catalysis close to real operating conditions, electrochemistry in real operating conditions, and development of sample environments. He obtained a Ph.D. in physics from Institut de NanoSciences de Paris, Université Pierre et Marie Curie (Paris, France) and was Marie Sklodowska Curie Fellowship at Diamond Light Source Ltd. (Oxford, UK). **f) References** 1. Bockris, J.O.M., A Hydrogen Economy. Science, 1972. 176(4041): p. 1323-1323. 2. Trimm, D.L. and Z.I. Önsan, Onboard Fuel Conversion for Hydrogen-Fuel-Cell-Driven Vehicles. Catalysis Reviews, 2001. 43(1-2): p. 31-84. 3. Jacobson, M.Z., W.G. Colella, and D.M. Golden, Cleaning the Air and Improving Health with Hydrogen Fuel-Cell Vehicles. Science, 2005. 308(5730): p. 1901-1905. 4. Møller, K.T., et al., Hydrogen - A sustainable energy carrier. Progress in Natural Science: Materials International, 2017. 27(1): p. 34-40. 5. Ajanovic, A., M. Sayer, and R. Haas, The economics and the environmental benignity of different colors of hydrogen. International Journal of Hydrogen Energy, 2022. 47(57): p. 24136-24154. 6.The 6th Strategic Energy Plan. https://www.enecho.meti.go.jp/en/category/others/basic_plan/. 7. Pivovar, B., N. Rustagi, and S. Satyapal, Hydrogen at Scale (H2 @Scale): Key to a Clean, Economic, and Sustainable Energy System. The Electrochemical Society Interface, 2018. 27(1): p. 47-52. 8. Council, H., Hydrogen scaling up: A sustainable pathway for the global energy transition. 2017. 9. Report, E.C. Charting the Energy Transition to 2050. 2022; Available from: https://www.ema.gov.sg/energy-2050-committee-report.aspx. 10. Ayers, K., High efficiency PEM water electrolysis: enabled by advanced catalysts, membranes, and processes. Current Opinion in Chemical Engineering, 2021. 33: p. 100719. 11. James Vickers, et al., Cost of Electrolytic Hydrogen Production with Existing Technology. 12. 4 technologies that are accelerating the green hydrogen revolution. https://www.weforum.org/ agenda/2021/06/4-technologies-accelerating-green-hydrogen-revolution/. 13. Emanuele Taibi, H.B., Raul Miranda, Marcelo Carmo, Dolf Gielen, Roland Roesch, Green Hydrogen Cost Reduction: Scaling up Electrolysers to Meet the 1.5ºC Climate Goal. International Renewable Energy Agency, 2020. 14. Hou, J., et al., Rational Design of Nanoarray Architectures for Electrocatalytic Water Splitting. Advanced Functional Materials, 2019. 29(20): p. 1808367.

	15. Jin, H., et al., Single-Crystal Nitrogen-Rich Two-Dimensional Mo5N6 Nanosheets for Efficient and Stable Seawater Splitting. ACS Nano, 2018. 12(12): p. 12761-12769. 16. Yang Yang et al. , O-coordinated W-Mo dual-atom catalyst for pH-universal electrocatalytic hydrogen evolution. Sci. Adv. 6, eaba6586 (2020) 17. L. Liu et al., Metal Catalysts for Heterogeneous Catalysis: From Single Atoms to Nanoclusters and Nanoparticles Chem. Rev. 2018, 118, 4981 18. Gao, Y., et al., Microenvironment Engineering of Single/Dual-atom Catalysts for Electrocatalytic Application. Adv. Mater. 2023 Accepted Author Manuscript 2209654. 19. Zhou, X., et al., Dual-Site Single-Atom Catalysts with High Performance for Three-Way Catalysis. Adv. Mater. 2022, 34, 2201859. 20. Wang, M., et al., Non-planar Nest-like [Fe_2S_2] Cluster Sites for Efficient Oxygen Reduction Catalysis. Angew. Chem. Int. Ed. 2023, 62, e202300826. 21. Mannix, A., Kiraly, B., Hersam, M. et al. Synthesis and chemistry of elemental 2D materials. Nat Rev Chem 1, 0014 (2017)

Joint Projects

Home University	Nanyang Technological University	
Supervisors	**Home**	**Partner**
Name	Assoc. Prof. Lee Jong-Min	Dr Axel Wilson
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Project Title	**Electrocatalyst Design through Modulating Dual-Atomic Coordination on Monolayered Elemental Substrates**	
Project Description (200-300 words)	Developing high-efficient electrocatalysts for water electrolysis and fuel cell applications is crucial to the pursuit of a sustainable energy future. Constructing electrocatalysts by rational design at the atomic level has been increasingly regarded as a promising approach thanks to recent advances in material characterization and theoretical comprehension. In particular, dual-atomic nanoarchitecture is gaining significant interest due to the enormous possibility of structure modulation toward realizing novel reaction mechanisms. In comparison to the state-of-the-art single-atom electrocatalyst, the presence of two active sites in close proximity enables strong synergism, leading to significantly enhanced catalytic performance. Furthermore, the controlled coordination of two atoms allows precise control over the reaction intermediates and reaction pathways, thereby improving the selectivity toward the desired products. Besides, the dual-atom configuration provides mutual support, preventing atom agglomeration or detachment during catalytic reactions and thus enhancing operational stability. Recently, various post-graphene 2D elemental materials have been developed, attracting substantial interest owing to the rich structural chemistry and enhanced anisotropic electron transport triggered by unique Fermi surface topography. More importantly, in contrast to carbon-based materials, the non-carbon elemental 2D materials feature strong interaction with metallic atoms, allowing electronic modulating and stabilizing of the dual-atom structures simultaneously. Herein, I hypothesize that the precise coordination modulating of dual-atomic moieties grown on monolayer elemental 2D materials will enable significantly enhanced catalytic performance. To explore the hypothesis, in this project, I will target three key objectives as follows • Devise a facile synthetic pathway to prepare dual atoms confined on monolayered elemental 2D substrates. • Characterize materials' chemistry, nanostructure, and	

	electrocatalytic performances. • Investigate the structure-function relationship using theoretical simulation and Operando studies. The developed electrocatalysts with high performance and excellent long-term stability would be further characterized in pilot scale for real-life applications. More importantly, this project will provide insightful guidance for the rational design of advanced electrocatalysts, facilitating the translation of scientific research to industrial applications.
Program/Center Website(s)	Laboratoire de Réactivité de Surface http://lrs.sorbonne-universite.fr/ Graduate College https://www.ntu.edu.sg/graduate-college
Additional Information (e.g., files with project details)	2023 Joint Program_Project Details.docx

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Joint Projects

Home University	Nanyang Technological University	
Supervisors	**Home**	**Partner**
Name	Rei KINJO	Jamal MOUSSA (Primary supervisor) Lydia Sosa Vargas Fabrice Mathevet
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Website	https://personal.ntu.edu.sg/rkinjo/index.html	https://ipcm.fr/index.php/recherche/presentation-equipe-arc/composition-de-lequipe-arc/jamal-moussa/
Project Title	**Merging Pyridylidenes and Main Group Element: From Highly Luminescent Molecules to Polymers and Applications**	
Project Description (200-300 words)	**Overview of the project:** This project involves both fundamental and applied chemistry aspects. The team of Sorbonne Université has recently developed new powerful methodologies of preparation of pyridylidene complexes. On the other hand, a variety of p-block elements-based aromatic heterocycles have been developed by the team in NTU over the last years. By combining both research areas, this project aims to develop a new class of compounds incorporating p-block elements into the pyridylidene scaffolds, and elucidate their bonding and structural features as well as the optical properties. Furthermore, the luminescent properties of those compounds will be examined and modified which may lead to the potential application in the preparation of novel OLEDs. (NTU primary contribution) (i) The synthesis, spectroscopic characterization, structural authentication of the main group elements-incorporated pyridylidene building blocks. (ii) The screening of the basic reactivity of the developed compounds. (Sorbonne Universite primary contribution) (i) Development, spectroscopic characterization, elucidation of the photophysical & optical properties of the main group elements-incorporated pyridylidene oligomers/polymers. (ii) Preparation and assessment of OLEDs Theoretical analysis will be done by both NTU and Sorbonne Universite collaboratively.	

Program/Center Website(s)	NA
Additional Information (e.g., files with project details)	The candidate should ideally possess a strong background in synthetic organic and inorganic chemistry and/or organometallic chemistry with fundamental knowledge in optical properties (absorption and emission). Skills in polymer chemistry and DFT calculation methods would be a plus. The final compounds that exhibit important and are adequate will be used to prepare OLEDs in the laboratory of Prof. Adachi at Kyushu University, JAPAN.