CHEMICAL ENGINEERING
UNIVERSITY of WASHINGTON

SEMINAR

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Bridging Physics-Informed and Data-Driven Materials Designs for Deep Decarbonization

Monday July 31st
Lecture 4:00-5:00 p.m. | Physics/Astronomy Auditorium (PAA) A110
Reception 5:00-6:00 p.m. | Benson Hall Lobby

Bio

Dr. Jiayu Peng is a postdoctoral associate in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology, supervised by Prof. Rafael Gómez-Bombarelli. He obtained his Ph.D. in Materials Science and Engineering in 2022 from the same department working with Prof. Yang Shao-Horn, and his B.Sc. in Applied Physics from the University of Science and Technology of China in 2017. Jiayu has been awarded the Graduate Student Award from the Materials Research Society and featured by the inaugural ENFL Future Investigator Spotlight from the Energy and Fuels Division of the American Chemical Society. His research bridges physics-informed and data-driven materials designs to electrify and decarbonize chemical transformations and energy storage combining physical chemistry, material descriptors, atomistic simulations, advanced characterizations, and machine learning. He aims to build a diverse, inclusive research program that empowers all to collectively construct non-conformist solutions to combat the most recalcitrant societal challenges—climate change, pollution, energy poverty, and food insecurity.

DYSS2023

Abstract

Electrifying and decarbonizing the chemical industry is a pressing chemical engineering mission of our time. The chemical industry is the world's biggest energy consumer and the third-largest source of emissions, where the overproduction of CO2 has led to severe problems such as global warming. To tackle these issues, governments and industrial players worldwide have set ambitious targets to reduce carbon emissions. For example, the current U.S. administration aims to half the emissions of 2005 by 2030 to reach net zero by 2050. To facilitate such deep decarbonization, it is crucial to electrify the chemical industry—transforming earth-abundant molecules into green chemicals and fuels using electricity converted from solar and wind energy. A core element in achieving this goal lies in developing novel clean energy technologies enabled by unprecedented materials (e.g., catalysts).

Unfortunately, there is no time left for materials design as usual, as inventing new materials is a painstakingly slow process. On average, previous innovations have taken 20 years to discover a material and bring it to market. To accelerate materials design for deep decarbonization, it is imperative to bypass traditional research paradigms that rely too heavily on tedious trial and error, unsystematic chemical intuition, and pure serendipity.

To this end, I will introduce how a joint computational–experimental approach can be established to develop physics-informed and data-driven blueprints to boost materials design for decarbonization by combining physical chemistry, material descriptors, atomistic simulations, advanced characterizations, and machine learning.

As an example, I will highlight my work on building quantitative physics-informed design principles of catalyst materials to optimize their reactivity and durability for catalyzing electrochemical water oxidation. Notably, I have combined electrochemistry and reaction kinetics with first-principles atomistic simulations and synchrotron X-ray spectroscopies to unveil how to mechanistically understand and quantitatively engineer these materials to realize optimal activity and stability. I have elucidated how rationally controlling the electronic structure of transition metal compounds can effectively tune their chemical bondings, modulate key reaction barriers, and thus optimize their reactivity and durability, offering quantitative predictive power to boost materials design for decarbonization.

I will also show how materials design can be further accelerated by coupling physics-based design principles with machine learning. I will focus on multicomponent oxides—an uncharted class of materials with great promise for decarbonization but with too-high structural complexity (e.g., cation orderings) for an exhaustive investigation. To conquer this challenge, I have built data-driven ordering descriptors that universally rationalize and accurately predict experimental cation orderings in these complex oxides. Furthermore, I have developed equivariant graph neural networks to accurately predict key cation ordering–dependent properties by learning intrinsic symmetries, enabling efficient discoveries of new multicomponent oxides over a design space of up to billions of materials.

To conclude, I will pinpoint challenges and opportunities in further unlocking transformative materials design for fully electrifying and decarbonizing chemical transformations to bring qualitative changes to the world.