CHEMICAL ENGINEERING
UNIVERSITY of WASHINGTON

SEMINAR

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Physics-Informed Machine Learning Frameworks for Material Discovery

Monday August 21st
Lecture 4:00-5:00 p.m. | Physics/Astronomy Auditorium (PAA) A110
Reception 5:00-6:00 p.m. | Benson Hall Lobby

Bio

Dr. Maitreyee Sharma Priyadarshini is a Postdoctoral Research Associate with Prof. Paulette Clancy and Prof. Rigoberto Hernandez at Johns Hopkins University. She currently works on developing computational material discovery algorithms and multi-scale material models for energy and space applications. Before this, Maitreyee completed her Ph.D. in Aerospace Engineering at the University of Illinois, Urbana-Champaign, advised by Prof. Marco Panesi. Her thesis work focused on developing a computational framework to accurately predict and mitigate heating on spacecraft surfaces. Maitreyee's work has been recognized by multiple awards and honors, including Aerospace Engineering Alumni Advisory Board Fellowship (UIUC), Rising Stars in Aerospace (MIT), Mavis Future Faculty Fellowship (UIUC), and Outstanding Asian & Asian American Graduate Student Leader Award (UIUC). She is firmly committed to enhancing diversity, equity, and inclusion in STEM through mentoring, outreach, and service activities. Apart from research, she loves dancing and teaching dance. She has trained in Bharatnatyam, an Indian classical dance form, for over 20 years. She also enjoys practicing yoga and swimming.

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Abstract

The lack of efficient discovery tools for advanced functional materials is a major bottleneck to enabling next-generation energy, health, space, and sustainability technologies. One main factor contributing to this in- efficiency is the large combinatorial space of candidate materials which is very sparsely observed. Moreover, searches of this large combinato- rial space are often biased by expert knowledge and clustered close to material configurations that are known to perform well. Experimental characterization and first principles quantum mechanical calculations of all possible materials are extremely expensive leading to small data sets not suitable for a number of approaches, such as Deep Learning. As a result, there is a need for computational algorithms that can efficiently search this large space.

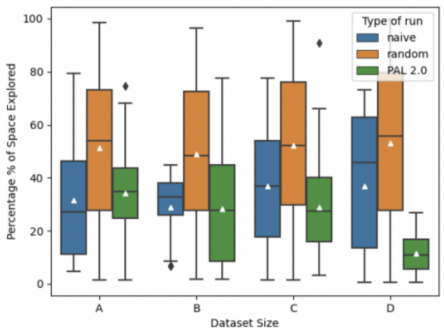

Figure 1: Performance of the PAL 2.0 on discovery of metal halide perovskite solar cell materials (A,C,D) and thermoelectric semiconductor materials (B).

In this talk, I will introduce a class of methods that combine physics-informed belief models with Bayesian optimization (BO). A material is characterized by physical and chemical properties of components of the material in a complex manner but a priori knowledge of the identity of the important properties is often lacking. The first part of my talk will introduce, PAL 2.0 [Romiluyi, Sharma et al, in preparation]. The key contributing factor of our proposed framework is in the creation of a hypothesis space with all possible Gaussian process representations of the domain using these different elemental/molecular properties and the ability to select the hypothesis (belief model) that best represents our material design domain. The best hypothesis is then used to perform a search of the material space. Our method is unique since it picks out the physical descriptors that are most representative of the material domain making the search unbiased toward expert knowledge, which in many cases is unknown. The model also provides valuable chemical insight into the domain that can be used to develop new materials that were outside the domain that was initially searched. Some applications of PAL 2.0 that I will discuss during my talk include perovskite solar cell and thermoelectric semiconductor materials, fig. 1. The second part of my talk will focus on material discovery algorithms for alloys which combine the PAL 2.0 methodology with Gaussian Process-Neural Network (GP-NN) models [Clancy, Nam, Sharma, HEMI Seed Grant, 2023]. The novel combination of GP-NN+BO algorithm makes use of the generalization power of Deep learning models [Sharma et al, PCCP, 2023] and the exploratory power of the BO algorithm at a minimal computational cost. Results shown in fig. 2 demonstrate the out-performance of the GP-NN model which on average explores just 15% of the space to find the optimal solar cell material. Overall, by accelerating discovery for materials like high-entropy shape memory alloys, space solar cell materials and thermoelectrics, these methods will enable creation of large data sets for various material classes that can then be leveraged in training deep learning models for property predictions and multi-scale modeling.

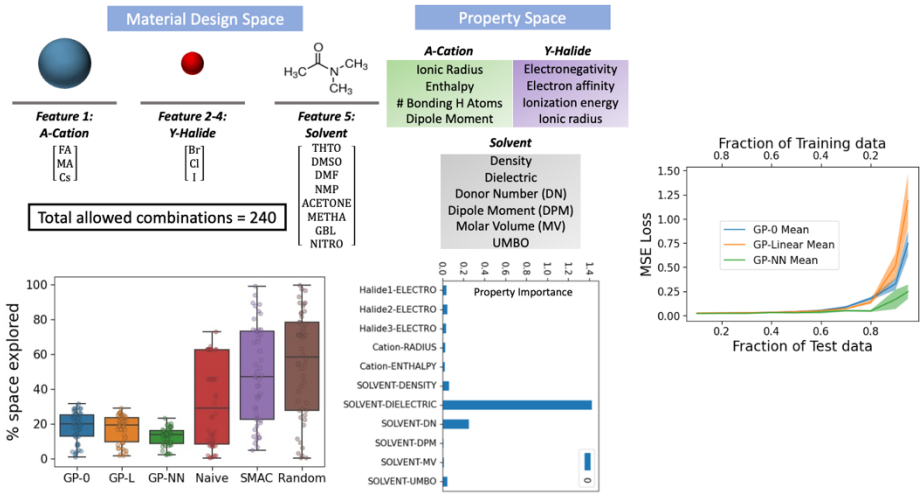

Figure 2: Performance of the GP-NN method on discovery of metal halide perovskite solar cell materials.