PCSI

Room Redondo - Session PCSI-MoE

Novel Materials

Moderator: Christopher Palmstrøm, University of California, Santa Barbara

7:30pm **PCSI-MoE-1 Machine Learning in the Quantum Regime Through Physical-Principle-Informed Representations***, **Qimin Yan**,* Department of Physics, Northeastern University **INVITED**

Materials design in the quantum regime call for the integration of multi-tier materials information that goes beyond atomic structures. Especially, many quantum behaviors are greatly controlled by local bonding environments and physical constraints related to symmetry. In this talk, I will give several examples of how domain knowledge and physical principles for quantum material systems can be incorporated into machine learning frameworks through representation learning to greatly improve the performance of machine learning models for property predictions. Motivated by Pauling's rules, I will show that local bonding environments (structure motifs) can be incorporated into a graph-based machine-learning architecture to make reliable property predictions for solid-state quantum materials including complex metal oxides. The proposed atom-motif dual network model demonstrates the feasibility to incorporate beyond-atom materials information in a graph network framework and achieves state-of-the-art performance in predicting the electronic structure properties of complex metal oxides. Through unsupervised learning, abstracted material information such as chemical formulas and motif connections can be combined with national language processing technologies to effectively represent fundamental elements in materials and use them in downstream learning tasks. I will demonstrate how contrastive representation learning can be used to incorporate physical constraints that control the collective behavior of electron densities into neural-network-based density functional design. At the end of the talk, I will discuss the continued development of machine learning models for quantum materials that embrace local/global symmetries and symmetry-based interactions.

8:10pm **PCSI-MoE-9 UPGRADED: Ultra-Thin Freestanding Membranes Enables New Discovery of Interfacial Properties***, **Xiao Zhao**, Y. Lu, M. Salmeron,* LBNL

Many surface-sensitive techniques have been improved recently to narrow the gap between measuring environmental conditions from vacuum to practical gas and liquid environments. To extend the pressure range and to enable measurements of the liquid phase, thin film membranes acting as windows in environmental cells have been fabricated. Herein, we present a new generation of ultrathin free-standing membranes made with graphene, oxide films (2-10nm Al_2O_3, TiO_2, etc.) or metal (3-10nm Pt)[1]. The films are mechanically robust and transparent to electrons and photons. Their applicability for various environmental spectroscopies, such as X-ray Photoelectron Spectroscopy (XPS, 1bar for gas or for liquid), Infrared Nanospectroscopy (nano-FTIR, solid-liquid interface), Kelvin Probe Force Microscopy (KPFM) and Sum Frequency Generation (SFG) is demonstrated[1,2]. With this platform we investigated the structure and profile of electrical double layer, self-assembly of protein and electrocatalyst evolution. The remarkable properties of such ultra-thin membranes open up broad opportunities for atomic/molecular level studies of interfacial phenomena (corrosion, catalysis, electrochemical reactions, energy storage, geochemistry, and biology) in a broad range of environmental conditions.

8:30pm **PCSI-MoE-13 UPGRADED: Extreme Spatiotemporal Imaging and Control of Nanophotonic Components and Their Neuromorphic Applications***, L. Wittenbecher, D. Winge, A. L'Huillier,* Lund University, Sweden*; J. Vogelsang,* Oldenburg University, Germany*; D. Zigmantas,* Lund University, Sweden*; **A Mikkelsen**,* NanoLund and Department of Physics, Lund University, Sweden

During the past decade we achieved unprecedented abilities to probe and exploit light-matter interaction down to the nanometer and sub-femtosecond spatiotemporal scales. This opens for new fundamental physical insights as well as to rationally design of a variety of novel functional materials and devices with applications for energy harvesting and alternative computing. The presentation has two parts:

First, we combine the femtosecond and attosecond time resolution of advanced laser systems with the nanoscale spatial resolution of PhotoEmission Electron Microscopy (PEEM). We use this to unravel the hot electron dynamics in InAs nanowires [1] and observe the dynamics of near-field enhancement in hybrid metal-semiconductor nanostructures [2,3]. We will include new works using very high fields on Ag nanowires and attosecond pulse excitation on ZnO.

Second, we propose an artificial neural network concept [4] in which the weighted connectivity between nodes is achieved by overlapping light signals inside a shared quasi 2D waveguide – a broadcasting concept. This decreases the circuit footprint by two orders of magnitude compared to existing optical solutions. The evaluation of optical signals is performed by neuron-like nodes constructed from efficient III–V nanowire optoelectronics. This minimizes power consumption of the network. Detailed simulations of the central network parts, demonstrate feasibility [4] and new experimental data on wire-to-wire on chip communication circuits will be shown.

[1] L. Wittenbecher et al, ACS Nano 15 (2021) 1133.

[2] J. Vogelsang, ACS Photonics 8 (2021) 1607

[3] J.H. Zhong, et al. Nature Communications 11 (2020) 1

[4] D. O. Winge, et. al ACS Photonics 7 (2020) 2787

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