PCSI
Room Redondo - Session PCSI-SuE
Characterization Methods
Moderator: Chip Eddy, Jr., ONR Global

7:30pm **PCSI-SuE-1 Atomic Scale Structural Characterization of Material Surfaces and Interfaces via Atomic Electron Tomography*, Yongsoo Yang,*** Korea Advanced Institute of Science and Technology, Republic of Korea **INVITED**

A high degree of anisotropy and even completely new phenomena can be often found at the materials surface/interface systems, and their properties are governed by the 3D arrangement of individual atoms at the surface/interface. To achieve a proper understanding of structure-property relations at the interface, a precise determination of the 3D interface atomic structures and their dynamics is a definite prerequisite, which has been limited to lower-dimensional measurements or simulations. Traditional crystallography, which is reliant on periodicity, cannot determine their real structures because the periodic symmetry breaks down at the surface/interface. Without any prior assumption of underlying structure, atomic electron tomography (AET) is now able to locate the 3D coordinates of individual atoms and their dynamics with picometer precision and with elemental specificity. A variety of complex internal atomic structures can be measured with 3D atomic-level details; including grain boundaries, chemical order/disorder and phase boundaries [1]. Recently, combined with deep-learning based neural network, it now became possible to precisely measure the 3D surface/interface structure of nanomaterials with high precision, revealing surface-substrate boundary effect, coalescence dynamics, core-shell strain relation and surface catalytic activity at the atomic scale [2-4]. Understanding the atomic resolution structural properties and their dynamics at the nanomaterial interfaces together with the relationship between atomic structure and material properties will allow the rational design of novel materials with desired surface/interface properties at the atomic scale.

[1] Y. Yang et al., Nature 542, 75 (2017).

[2] J. Lee, C. Jeong and Y. Yang, Nat. Commun, 12, 1962 (2021).

[3] J. Lee, C. Jeong, G. Lee, S. Ryu and Y. Yang, Nano Lett. 22, 665 (2022).

[4] H. Jo et al., arXiv:2207.06677 (2022).

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8:10pm **PCSI-SuE-9 Understanding Interface Effects in Van der Waals Heterostructures with Neutron Reflectometry*, Alex Grutter,*** National Institute for Science and Technology (NIST) **INVITED**

Layered Van der Waals (VdW) systems are among the most exciting playgrounds in condensed matter physics and include topological insulators, Weyl and Dirac semimetals, and 2D magnetic systems. In particular, heterostructures incorporating different classes of topological or magnetic orders are promising platforms for next generation quantum and spintronic devices. However, these systems represent a difficult materials engineering challenge in which reactive, often easily oxidized, materials must coexist and interact across sharp interfaces while preserving the target properties. It is in this context that simultaneous magnetic and structural depth profiling with polarized neutron reflectometry (PNR) has drawn considerable interest. With sub-Ångstrom resolution, sensitivity to magnetic signals originating within a single atomic monolayer, and the ability to detect chemical changes with precision, PNR is a powerful and non-destructive tool for probing low-dimensional nanostructures.

In this talk, we will introduce the basic concept of neutron reflectometry and use a series of recent examples to explore the unique insights PNR provides into the chemical and magnetic properties of VdW interfaces. Specifically will show how PNR identifies changes in surface chemistry, low-dimensional magnetism, magnetic proximity effects, and other forms of magnetic interface coupling in systems such as perovskite membranes, $(Bi,Sb)_2Te_3$, $MnBi_2Te_4$, $CrTe_2$, and Cd_3As_2.[1-7] Special emphasis will be placed on multimodal characterization approaches combining PNR with X-ray scattering, spectroscopy, muon spin relaxation spectroscopy, and electron microscopy for an even more comprehensive picture of the interface. By decomposing the magnetic and electronic properties on a layer-by-layer and element-resolved basis, new quantum material systems may be robustly understood and designed. We will conclude with a discussion on the future of ultra-sensitive magnetic interface probes and the potential impact from highly multiplexing neutron instrumentation such as a CANDOR reflectometer currently being commissioned at NIST.

References:

1. C.-Y. Yang et al., Science Advances 6, eaaaz8463 (2020)
2. W. Yanez et al., Physical Review Applied 16, 054031 (2021)
3. N. Bhattacharjee et al., Adv. Materials 34, 2108790 (2022)
4. L. J. Riddiford et al., Phys. Rev. Lett. 128, 126802 (2022)
5. P. Deng et al., Nano Letters 22, 5735 (2022)
6. Q. Lu et al., ACS Nano 16, 7580 (2022)
7. P. Chen et al., Nat. Electronics *In Press* (2022)

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