PCSI
Room Keahou I - Session PCSI-SuA1
Materials for Novel Information Systems
Moderator: Dominik Zumbuhl, University of Basel, Switzerland

2:30pm **PCSI-SuA1-1 Interfacing Biomolecules with Coherent Quantum Sensors***, Peter Maurer, **Guanming Lao**,* University of Chicago **INVITED**

Quantum metrology enables some of the world's most sensitive measurements with potentially far-reaching applications in the life sciences. Although the ultrahigh sensitivity of qubit sensors has spurred the imagination of researchers, implementation in actual devices that enable monitoring cellular processes or detecting diseases still remains largely elusive. Overcoming limitations that hold back wider application of quantum technology in the life sciences, requires advances in both fundamental science and engineering. In this talk, I will discuss our research group's recent results on addressing one of these long-standing research challenges, namely, how to interface highly coherent quantum sensors with biological target systems.

My discussion will start with the development of a novel biocompatible surface functionalization architecture for highly coherent diamond crystals. I will then continue with discussing a new approach to engineering spin coherence in core-shell structured diamond particles, which can be readily chemically modified and delivered to intact biological systems. Finally, I will conclude my talk with an outlook on a novel class of protein-based qubit sensors that will overcome many of the fundamental challenges associated with current diamond-based quantum sensors. The unifying theme of these advances are the convergence of techniques from single-molecule biophysics, material science, and quantum engineering. Specific applications of the developed sensing platforms to questions in the life sciences will be discussed throughout this talk.

3:10pm **PCSI-SuA1-9 Magnetoresistance Spectroscopy of Near-Surface Defects in Semiconducting Hosts***, **Stephen McMillan**,* Donostia International Physics Center, Spain **INVITED**

Components for quantum information processing and quantum sensing require localized spin-coherent states. These states can be realized in isolated magnetic dopants embedded in a non-magnetic semiconducting host. A critical requirement for utilizing a dopant-based system is an understanding of how the complex host environment influences the coherent spin dynamics at an individual site. Resolving these faint dynamics against a strong incoherent background is a challenge that is typically solved by exciting the system via ac fields. In this work we propose a method that leverages non-equilibrium spin correlations in the presence of dc magnetic fields to probe coherent interactions in individual near-surface magnetic dopants. In previous work, we calculate the dc magnetoresistance through a spin-1/2 dopant that is addressed by a spin-polarized scanning tunneling microscope (SP-STM) and exchange coupled to an inert spin-1/2 center [1]. This work is then extended to the technologically relevant case of an individual spin-1 center [2]. In particular we use the stochastic Liouville formalism to calculate the current through a divacancy in 4H-SiC. We predict distinct few-milli-tesla-dc magnetoresistance signatures that identify a single spin-triplet center's character and reveal the orientation of the spin triplet's zero-field splitting axis relative to the magnetic contact's polarization. For example, in 4H-SiC the single (*hh*), (*kk*),(*hk*), and (*kh*) divacancies are all distinct. Spin-polarized current flow efficiently polarizes the spin, potentially electrically initializing spin-triplet-based qubits without the use of ac fields or optical hardware.

3:50pm **PCSI-SuA1-17 Development of 'Artificial' Memristive Synapses Using Various Sp2 C (Graphene-Like) -Sp3 C (Diamond) Heterojunctions as Neuromorphic Devices***, **Sanju Gupta**,* Gdansk University of technology and Penn State University*; R. Bogdanowicz,* Gdansk University of Technology, Poland

The integration of allotropic sp^2-/sp^3-bonded carbon (sp^2C/sp^3C) interfaces and devices has evoked increasing attention since they offer a versatile and rich playground for carbon-based electronics, electrochemical sensing platforms, and optoelectronic neuromorphic computing attaining enhanced performance [1-5]. Moreover, inspired by human brain functionality and its low power consumption of only 10W, memristors for neuromorphic computing have gained significance for implementing solid-state neurons and 'artificial' synapses due to their nanoscale footprint and reduced complexity. In this talk, we present the fabrication of various carbon-based heterojunctions comprising graphene-like (sp^2C)-diamond (sp^3C) architectures using microwave plasma-assisted chemical vapor deposition on nanodiamond seeded *p*-Si (100), SiO_2/*p*-Si (100) and *Fz*-Si (001) substrates. These are the key elements emulating the characteristics of biological synapses and memory functions which are game-changing energy-saving computing devices. The resulting heterojunctions behave as memristors (*i.e.,* resistors with tunable memory) having multiple resistance states and nonvolatile memory functions, a phenomenon that refers to the ability of synapses (neuronal links) to adapt in response to an increased or decreased activity, essential to human memory and learning. The resulting heterojunctions behave as memristors (*i.e.,* resistors with tunable memory) having multiple resistance states and nonvolatile memory functions, a phenomenon that refers to the ability of synapses (neuronal links) to adapt in response to an increased or decreased activity, essential to human memory and learning. We performed *I–V* characteristics with temperature (up to 250 ^oC) and in response to photoirradiation at 365 nm, 532 nm, and 633 nm in addition to comprehensive microstructural properties. Interestingly, high or low resistance states (equivalently, short-term, and long-term potentiation) can be controlled by combined applied bias and light irradiation, giving a resistive switching ratio of ~10^6, observed in sparse materials and/or heterostructures. They exhibit quasi-linearity and symmetry when subjected to identical input pulses, essential for their role in the online training of neural networks. The linearity holds for a range of pulse width, amplitude, and applied pulse number. We ascribe the observed behavior to redox reaction (or reorganization of carbon orbitals) at the sp^2-sp^3 interfaces and the role of hydrogen and oxygen movement by applied bias. Finally, heterostructure arrays could be designed for better memristive devices and memory functions and photo sensing (image sensors) applications.

3:55pm **PCSI-SuA1-18 In-Situ Transmission Electron Microscopy of Hafnium Zirconium Oxide for Phase Identification in Memristor Devices***, **Krishnamurthy Mahalingam**,* BlueHalo-UES Inc*; Shiva Asapu,* Department of Electrical and Computer Engineering, University of Massachusetts*; Larry Blank,* ARCTOS Technology Solutions*; Derek Winner,* University of Dayton*; Cynthia Bowers,* Blue Halo-UES Inc*; Sabyachi Ganguli, Ajit Roy,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Joshua Yang,* Department of Electrical and Computer Engineering, University of Southern California

Hafnium zirconium oxide (HZO) has attracted much attention for the development of memristive technologies essential for neuromorphic computing, which is based on ferroelectric switching behavior attributed to orthorhombic polar phase (OPP) formation. This phase is stabilized by thermal strain induced by electrode type and process conditions. However, due to the polymorphic nature of HZO, formation of other stable polycrystalline phases with monoclinic, tetragonal and cubic structure is also possible. The identification of the crystalline phases by standard techniques is achallenge due to the similarity of lattice parameters and symmetry along some orientations, making it difficult for insightful optimization of OPP formation in these devices.

Herein we performed in-situ transmission electron microscopy, combining electron energy loss spectroscopy (EELS) and position averaged convergent beam electron diffraction (PACBED) to directly examine amorphous to crystalline phase transformation in HZO films under rapid thermal annealing. In EELS the signatures to identify the different phases was investigated by a detailed examination of the fine structure near the O_K edge. In PACBED we combine dynamical diffraction simulations with neural network based machine learning (ML) to examine distinction between the different phases. A high resolution TEM image of the crystalline phase formation is presented in Fig. 1(a) along with an inset showing its digital fast Fourier transform after rapid heating to 700^{o}C (at 50^{o}C/sec). Figure 1(b) is an EELS profile comparing the O_K edge from an amorphous region (Blue) before and the crystalline region (Red) after the annealing operation. Noticeable shift in peak-B position and a reduction in the B/A peak ratio are evident. While conventional diffraction analysis confirmed the formation of OOP, application of ML was inconclusive. Further details on the interpretation of changes in the O_K edge fine structure based on EELS modeling, and challenges with the ML approach to electron diffraction data analysis will be presented.

4:00pm **PCSI-SuA1-19 Quantum Sensing Using Two-dimensional Hexagonal Boron Nitride***, **Hailong Wang**,* Georgia Institute of Technology, USA

Emergent color centers with optically accessible spins have attracted tremendous research interest in recent years due to their significant potential for implementing transformative quantum sensing technologies. Spin defects hosted by hexagonal boron nitride (hBN) are emerging candidates in this catalog due to their remarkable compatibility with solid-state nano device integration and multimodal sensing of proximal two-dimensional quantum materials/devices [1]. Taking advantage of boron vacancy spin defects in hBN, we report nanoscale quantum imaging of low-dimensional ferromagnetism sustained in Fe_3GeTe_2/hBN van der Waals heterostructures [2]. Exploiting quantum spin relaxometry methods, we have observed spatially varying magnetic fluctuations in exfoliated Fe_3GeTe_2 nanoflakes, whose magnitude reaches a peak value around the Curie temperature. Using optically detected magnetic resonance measurements, we further show that ferromagnetic resonance and parametric spin excitations in a magnetic insulator $Y_3Fe_5O_{12}$ (YIG) can be effectively detected by boron vacancy spin defects under various experimental conditions through the off-resonant dipole interaction between YIG magnons and boron vacancy spin defects [3]. Our results highlight the opportunities offered by novel quantum spin defects in layered vdW materials for investigating microscopic spin behaviors in magnetic solid-state matters.

[1]A. Gottscholl et al., Nature Materials **19**, 540 (2020).

[2]M. Huang et al.,Nature Communications**14**, 5259 (2023).

[3]J. Zhou et al., Science Advances **10**, eadk8495 (2024).

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