PCSI

Room Canyon/Sugarloaf - Session PCSI-2MoM

Hybrid Materials

Moderator: Joseph Berry, National Renewable Energy Laboratory

11:00am **PCSI-2MoM-31 Hybrid Perovskite-Based High Energy Photon Detectors**, ***Wanyi Nie,*** Los Alamos National Laboratory **INVITED**

Radiation spectroscopy is widely needed in security, medical treatment, nuclear material monitoring as well as space science. It quantifies the gamma-ray energies by single radiation photon counting devices. The key is to precisely count gamma-ray photons using highly sensitive detectors. Solid-state detectors employing high density semiconductors to convert gamma-ray photon signal directly into electrical pulses offers promising solution. It outperforms scintillator technologies in count rate and sensitivities with high energy resolutions.

In this talk, I will introduce our recent progress on methylammonium lead halide perovskite single crystal detectors. We show that the single crystal detectors can efficiently count single gamma-ray photon events with electrical pulses. We further investigate the operational principles of the bromide-perovskite solid-state detectors and find using high work function contacts can block out the dark noise from thermally injected electrons and thus allow for efficient pulse collection at higher electrical fields. As a result, we observe strong and reproducible electrical pulses when exposing the detector under several radioactive sources corresponding to gamma-rays at various energies. However, we also discover that the bromide-perovskite detector suffers from voltage instability and slow response which cannot generate reliable energy resolved spectrum. Replacing the bromide by iodide in the crystal, we are able to operate the detector at much higher voltage and deliver sharp electrical pulses at room temperature. By counting the pulses under gamma-ray photons, we constructed the spectrum for ^{137}Cs that clearly shows the expected Compton scatter structure along with signals from photo-electric effect. Our results lay the foundation towards the robust operation of efficient perovskite- detector.

11:40am **PCSI-2MoM-39 Pb-based Metal-Organic Frameworks for Efficient Perovskites Light-emitting Diodes Applications**, ***Hsinhan Tsai,*** *W Nie,* Los Alamos National Laboratory

Hybrid perovskites materials have demonstrated an extraordinary potential for clean, sustainable energy technologies and low-cost optoelectronic devices. In spite of the unprecedented progress in photovoltaics over the past decay, perovskites light-emitting diodes (PeLEDs) emergent as one of the most promising light emitters with performances exceeded 20% EQE efficient and low energy consumption devices. One of the key challenges that exists in the field today is the stability and reliability of devices under operation conditions. This vulnerability remains an open question, which might determine the fate of this remarkable material despite excellent properties.

A fundamental requirement for achieving highly efficient light emission and stability operation used in PeLEDs is to design molecular structures that facilitate recombination of the electrically or optically generated electron and hole pair to emit photons. Here, we demonstrate a new type Pb-based metal-organic frameworks (MOFs) perovskites as LED emitter with naturally formed quantum and dielectric confinement, where efficient radiative recombination is expected. We show that the Pb-based MOFs have a PeLEDs performance with over 5% EQE and extended charge localization due to the structure confinement and consequently improved the carrier transport and radiative recombination.

[1] Zhao et al, *Nat. Photonics*, **12**, 783–789 (2018).

[2] Xu et al, *Nat. Photonics*, **13**, 418–424 (2019)

[3] Tsai et al, *Adv.Mater.,* **30**, 1704217 (2018).

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11:45am **PCSI-2MoM-40 Arrangement and Electronic Properties of Cobalt Phthalocyanine Molecules on B-Si(111)-√3 × √3 *R* 30°**, ***Susi Lindner,*** *M Franz, M Kubicki, S Appelfeller, M Dähne, H Eisele,* Technische Universität Berlin, Germany

The molecular arrangement and the interfacial electronic properties of cobalt phthaloycyanine (CoPc) on the deactivated B-Si(111)-√3 × √3 *R*30° surface are analyzed using scanning tunneling microscopy and spectroscopy as well as photoemission studies. Our data demonstrate that for a low coverages of CoPc the molecules lie at with the p_z orbital of the Si surface atom forming a hybrid state with the d_{z2} orbital of the transition metal. This hybridization is observed in an additional contribution to the valence band spectrum. Furthermore, this additional hybridization state is detected in the tunneling spectrum. For higher CoPc coverages, the CoPc molecules are tilted with respect to the Si surface forming highly ordered organic molecular films. The spectroscopic data of the thick film demonstrates that the electronic properties resemble those of pure CoPc.

11:50am **PCSI-2MoM-41 Amino-Acids Detection with Modulation Doped and Surface Nanoengineered GaAs Schottky Diodes**, *T Alkhidir, M Abi Jaoude,* KUST, United Arab Emirates; *D Gater,* University College London, United Kingdom; *C Alpha,* Cornell University; ***Abdel Isakovic,*** Colgate University

Most current techniques for analyzing amino acids require substantial instrumentation and significant sample pre-processing. We designed, fabricated and tested scalable diode-based microdevice that allows for direct sensing and quantification of amino acids. The device is based on modulation doped GaAs heterostructure with a Schottky contact on one side. While relatively high mobility and small dielectric constant of GaAs are naturally helpful in this problem [1][2], we present how etching procedure allows for substantial modification of the surface properties, thereby further boosting the sensing performance. We present data for several qualitatively different amino acids (e.g. belonging to different classes, such as non-polar with aliphatic R-group, polar uncharged R- and charged R-group) with specific examples of Glycine, Cysteine and Histidine, respectively.

The conductance for the GaAs-amino acid interface measured using scanning tunneling microscope (STM) was previously reported to have distinct spectral features [3][4]. In this talk, we show that measuring differential conductance of GaAs diode whose surface is in a direct contact with an amino acid, can still lead to a useful (and easier to obtain) information, previously available only via effective but cumbersome STM and molecular electronics type of approaches. We employ standard multivariate data analysis techniques extract reliably distinct (> 97%) single amino acid specific features. We also present how sensitivity of detection can be achieved within broadly varied pH levels (pH from 4 to 9, so far). Density functional theory (DFT) was used to examine which adsorption processes were likely responsible for surface conductance modification.

[1] M. Matmor and N. Ashkenasy, J. Am. Chem. Soc. **50**, 132 (2012).

[2] D. Bavli *et al*., Langmuir. **28**,1020 (2012).

[3] W. Shinwari *et al*., Adv. Funct. Mater. **20**, 1865 (2010).

[4] F. Piguet *et al*., Nat. Commun. **9**, 966 (2018).

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11:55am **PCSI-2MoM-42 Carrier Collection and Transport at Interface of Lead-FreeHalide Perovskites (FA,MA)SnI$_3$ Solar Cells**, ***William Jo,*** Ewha Womans University, Republic of Korea

Charge extraction at carrier transport layers adjacent to perovskites is crucial for the optimization of perovskite solar cells. In particular, Sn–perovskites with no lead elements are known to struggle from charge extraction. Here, we report effects of organic ligands like FA and MA (FA = $HC(NH_2)_2^+$; MA = $CH_3NH_3^+$) on charge separation at the interface between electron transport layers and perovskites. TiO_2 mesoporous covering the tin-perovskites show significant changes in electronic structure and built-in potentials according to the ratio of FA to MA. Through a local probe with potential and current mapping, charge transport has been intensively examined. The best cell in this study is obtained as 5.37% at FA : MA = 3 : 1 with only iodine at the halide sites. Even though the value itself is not comparable with lead halides but it could pave a new direction to improve lead-free perovskite solar cells.

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