Live Session
Room Live-2 - Session LI-WeM2

Wednesday Morning Live Session II: Biological, Environmental Interfaces and New Directions in the AVS

Moderators: Sidney Cohen, Weizmann Institute of Science, Israel, Caitlin Howell, University of Maine

10:00am **LI-WeM2-1 Welcome and Opening Remarks***, **Sidney Cohen**,* Weizmann Institute of Science, Israel

Welcome to the AVS 67 Virtual Symposium. We hope you will enjoy the event!

10:05am **LI-WeM2-2 ASSD 2021 Peter M.A. Sherwood Mid-Career Professional Award Talk: Information from complexity - Making Sense of the Mess Created by ToF-SIMS**, ***Daniel Graham***[1]*,* University of Washington, Seattle*; M. Taylor,* Pacific Northwest National Laboratory*; L. Gamble,* University of Washington, Seattle **INVITED**

ToF-SIMS data from even simple surfaces is complicated. This complexity is a blessing and a curse as it encodes information about the structure and composition of surface molecules and presents a massive data processing challenge to decode this information from within the hundreds of spectral peaks present in a typical spectrum. This challenge is further complicated by the fact that modern ToF-SIMS instruments can produce sub-micron resolution images where each pixel contains a full mass spectrum. This imaging modality can be combined with sputtering beams to enable depth profiles of materials which can contain multiple images acquired throughout the depth of a material. The result of this is a chemically rich, spatially mapped data matrix containing information about the chemistry, location, structure and composition of surface species. Such data matrices can contain tens of thousands (2D data) to millions (3D data) of spectra taking up 10s to 100s of GB. The challenge then becomes how to process this data and extract the gems of information encoded within the fragmentation patterns of each spectrum. To address these issues many researchers have applied a wide variety of multivariate and other advanced data analysis methods to ToF-SIMS data in order to extract useful information that can be used to aid in materials characterization.

In spite of this complexity, ToF-SIMS has found wide application in the analysis of organic and biological materials as it presents a method that can provide specific chemical information and precise localization of surface compounds.This can be particularly useful in the analysis of biomaterials, where understanding of the surface chemistry is critical to device success, and in the analysis of cells and tissues where mapping chemical changes can elucidate information that can be useful in understanding disease progression and possibly prevention.

In this talk I will demonstrate how the application of multivariate, and other advanced analysis methods, can facilitate digesting ToF-SIMS data and extracting useful information that can help solve problems in organic and biological materials characterization.Examples will be shown from spectral and image analysis (2D and 3D), along with ways we have explored to enable the characterization of topographically challenging samples used in tissue engineering.In addition I will highlight the importance of sharing tools developed for this type of analysis and describe tools we have created to facilitate multivariate analysis throughout the scientific community.

10:25am **LI-WeM2-6 High Throughput Discovery of Novel Antiviral Polymers for Reducing SARS-CoV-2 Surface Transmission and Improving PPE***, **Xuan Xue**, J. Duncan, C. Coleman, J. Ball, C. Alexander, M. Alexander,* University of Nottingham, UK **INVITED**

Respiratory diseases caused by viruses have become a serious global public health concern. The ongoing COVID-19 global pandemic has threatened people's lives and impacted socioeconomical development since December 2019. To date, Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) appears to spread easily in droplets in the air and via surfaces. Following evidence of virus contamination of surfaces, the fomite transmission of respiratory viruses has been highlighted as a potential infection route in the pandemic. In addition, healthcare workers in the front line of the COVID-19 outbreak response are exposed to the risk of SARS-CoV-2 infection daily. Personal protective equipment (PPE) is their main defence against viral contamination and to eliminate viral transfer from infected patients. Antiviral effective PPE materials, that can be self-disinfected and ideally worn for prolonged time, need to be developed.

In our study, a range of commercially available PPE materials and common surface plastics have been evaluated using live virus in Biosafety Level 3 (BSL-3) laboratory to enable a recommendation of which existing polymers should be employed for optimal viral inactivation on PPE. Detachment assays using virus like particles (VLPs), which do not have an infection risk, were used to investigate secondary spreading of viruses invoked by movement and doffing of PPE with both liquid and air flow systems explored to mimic actual environmental conditions. The persistence of live SARS-CoV-2 on these surfaces were evaluated and compared under varied temperature and relative humidity conditions.

In order to develop new polymers for PPE and fomite transmission control, high throughput polymer microarrays developed at the University of Nottingham, were used to identify novel anti-SARS-CoV-2 polymer materials.

10:45am **LI-WeM2-10 Machine-Learning-Assisted Photonics***, Z. Kudyshev, A. Kildishev, V. Shalaev, **Alexandra Boltasseva**,* Purdue University, USA **INVITED**

We coupled adversarial autoencoder deep generative network with adjoined topology optimization technique to advance metasurface design. The proposed approach speeds up the optimization search of highly efficient metasurface designs and also provides unparalleled control over the compressed design space distribution. The latter fact assures scalability of the approach to highly-constrained optimization problems.

Nanophotonics can provide solutions to interdisciplinary challenges in energy [1], quantum IT [2] and other areas. Addressing multifaceted problems require highly-constrained optimization of the device design, due to inherent complexity and multi-disciplinary nature of any practical application. Conventionally, adjoint [3] and genetic [4] optimization methods have been used to address such optimization tasks. However, the computational power requirement of these methods scales up with the number of constraints. This fact substantially limits the applicability of conventional optimization techniques to real-life applications. Within this work, we merged the adjoint topology optimization technique with adversarial autoencoders (AAE) to achieve significant improvement in the optimization search of non-trivial nano-antenna-based metasurface designs [5]. Particularly, we demonstrated that the proposed approach ensures not only the efficient optimization search of high-performance metasurface designs but also provides unparalleled control over the compressed design space distribution. The latter fact assures scalability of the approach to highly-constrained optimization problems. To showcase AAE-assisted method, we optimized a metasurface thermal emitter for thermophotovoltaic (TPV) applications. Compared to an adjoint-based topology optimized design with 92% efficiency of the thermal emission reshaping, the proposed method provides three times speed-up and gives 98% efficiency. The proposed approach can be adapted to a broader scope of the problems in optics.

References

[1] S. Linic, P. Christopher, D. B. Ingram, "Plasmonic-metal nanostructures for efficient conversion of solar to chemical energy," Nature Materialsk, vol. 10, pp. 911-921, 2011.

[2] S. I. Bogdanov, A. Boltasseva, V. M. Shalaev, "Overcoming quantum decoherence with plasmonics," Science, vol. 364, pp. 532-533, 2019.

[3] J. S. Jensen, O. Sigmund, "Topology optimization for nano-photonics," Laser and Photonics Reviews, vol. 5, pp. 308-321, 2011.

[4] C. Forestiere, et al., "Genetically engineered plasmonic nanoarrays," Nano Letters, vol. 12, pp. 2037-2044, 2012.

[5] Z. A. Kudyshev, A. V. Kildishev, V. M. Shalaev, and A. Boltasseva, "Machine-Learning-Assisted Metasurface Design for High-Efficiency Thermal Emitter Optimization," arXiv Preprint arXiv:1910.12741, 2019.

11:15am **LI-WeM2-16 STM Measurements of Spin-Polarized Currents Carried by the Topological Surfaces States of SmB_6 Nanowires***, **Vidya Madhavan**,* University of Illinois at Urbana-Champaign **INVITED**

Incorporating relativistic physics into quantum tunneling can lead to exotic behavior such as perfect transmission via Klein tunneling, or apparent faster than light travel. In this talk I will describe an experiment that demonstrates `helical tunneling', a process where spin-polarized electrons can be transmitted in a nominally time-reversal invariant fashion. To do this we use nanofabrication techniques to attach SmB_6 nanowires to the end of scanning tunneling microscope tips. SmB_6 is a topological Kondo

[1] **ASSD 2021 Peter M. A. Sherwood Mid-Career Professional Awardee**

Insulator which has been proposed to be an ideal topological system with Dirac fermions naturally dominating the density of states near Fermi level. The SmB_6 nanowire tips are used to image the canonical spin density wave material, $Fe_{1.03}Te$, which hosts a bicollinear spin order with a Neel temperature of ~50 K. STM images show a superstructure with the periodicity of the antiferromagnetic order, indicating spin-selective tunneling from the nanowire. The antiferromagnetic order becomes invisible above 10 K, far below the Neel temperature, together with the diminishing topological surface states. We further confirm a smoking gun signature of spin current generated by Dirac fermions, i.e., the contrast reversal of the antiferromagnetic order at opposite bias voltages. These findings establish interacting topological systems like SmB_6 as ideal conduits for spin-polarized topological currents and reveal an unexpected and unexplored consequence of relativistic tunneling.

11:35am **LI-WeM2-20 Molecular Nanostructures on Metals vs. Graphene: Towards Preserving Functional Properties**, ***Meike Stöhr***, University of Groningen, Netherlands **INVITED**

To preserve the (functional) properties of either individual adsorbates or well-ordered molecular assemblies upon adsorption on solid surfaces, the molecule substrate interactions have to be generally relatively weak. This can be achieved by introducing a decoupling layer between (metallic) surface and molecules. Among others, thin insulating layers of either NaCl or a single layer of hBN have been shown to be very useful to this end. The chemical inertness and the low density of states near the Fermi level also make graphene a good choice as a buffer layer to decouple adsorbed molecules from the underlying (metallic) substrate. Importantly, this holds the promise to preserve the intrinsic properties of the adsorbed species such as magnetic or catalytic properties. On the other hand, molecular self-assembly on graphene can be also employed as a promising method for tuning the electronic properties of graphene (doping or band gap opening) on a macroscopic scale while for this purpose, the molecule graphene interaction has to be larger than a mere physisorptive one.

Here we will discuss the structural and electronic properties for 1,3,5-benzenetribenzoic acid on graphene/Cu(111), for which different coverage dependent assemblies were observed. [1] We could demonstrate that the underlying Cu surface influences the structural arrangement of the molecules. With respect to the electronic properties, angle-resolved photoemission spectroscopy measurements showed n-doping of graphene. For parahexaphenyl-dicarbonitrile (NC-Ph_6-CN) on graphene, we observed the arrangement of a close-packed structure with a peculiar shift of every 4th molecule independent of coverage. We concluded that the screening properties of graphene are responsible for this effect since such a shift was neither observed for the case of metallic substrates nor for the bulk phase. [2] Adding Cu adatoms to submonolayer coverage of NC-Ph_6-CN resulted in the formation of metal-organic coordination networks with varying arrangements in dependence of the stoichiometry between molecules and Cu atoms. With scanning tunneling spectroscopy we characterized the electronic properties and could identify differences between the different assembly structures. [3] On the basis of the self-assembly process of tetracyanophenyl porphyrins before and after coordination with Co-atoms on Au(111), the influence of molecular coverage on decoupling could be demonstrated. [4]

[1] J. Li et al., J. Phys. Chem. C 120 (2016) 18093; N. Schmidt et al., unpublished.

[2] N. Schmidt et al., Chem. Eur. J. 25 (2019) 5065.

[3] J. Li et al., J. Phys. Chem. C 123 (2019) 12730.

[4] B.D. Baker et al., J. Phys. Chem. C 123 (2019) 19681.

11:55am **LI-WeM2-24 BID 2020-2021 Early Career Awardee Talk: Molecular-Level Insights Into Novel Wet Adhesion Systems Found in the Natural World**, ***Joe Baio***[1], Oregon State University **INVITED**

From sticky frog tongues to the superhydrophobic cuticles of springtails - the natural world is full of novel materials. Recent developments of surface analytical methods now allow provide a means of characterizing the structure and arrangement of molecules at complex biological interfaces. Many animals have adapted to a range of environmental surfaces by evolving a wet adhesion process. Previous studies of these adhesion mechanisms have focused almost exclusively on the mechanical and kinematic aspects of adhesion, and not on the molecular interactions at the fluid – substrate interface. In the work presented here, we first probe the molecular interactions between the adhesive fluid taken from lady beetles (*Cocinella septempunctata*) on two model substrates (one polar and one non-polar) with vibrational sum frequency generation (SFG) spectroscopy. The resulting SFG spectra demonstrate that during adhesion to a polar surface, fatty acids within the fluid form a highly ordered layer at the substrate surface. While on a non- polar surface, the mechanism changes and some other hydrocarbon species present within the fluid orders at the interface. The discussion will then be expanded to include some recent experiments identifying the structure of the biomolecules that make up the wet adhesive mechanism molecules present at a frog's tongue. Frogs capture their prey with a highly specialized tongue. Recent studies indicate this tongue is covered with fibril-forming mucus that acts as a pressure sensitive adhesive. However, no analysis of the interfacial chemistry of frog tongue mucus has been performed.Previous studies of mucus from other animals suggest that mucus from a frog's tongue consists of mucins—serine-, threonine-, and proline-rich glycoproteins. Therefore, the authors expect to observe chemical bonds associated with glycoproteins, as well as fibrils formed at the mucus–tongue interface. To test this hypothesis, we collected both near-edge x-ray absorption fine structure (NEXAFS) microscopy images and SFG vibrational spectra from layers of mucus left after frog tongue strikes on cleaned glass slides. NEXAFS imaging demonstrates a uniform distribution of amide, hydroxyl, and carbon–carbon bonds across the mucus surface. SFG spectra reveal that glycoproteins are well-ordered at the mucus–tongue interface.

12:15pm **LI-WeM2-28 Closing Remarks and Thank You's**, ***Caitlin Howell***, University of Maine

Thank you for attending today's session! Please note that our afternoon sessions begin at 12:50 pm EDT. Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler.

[1] **BID 2020-2021 Early Career Researchers Award**

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