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POSTER ABSTRACTS

Dilpuneet Aidhy

Machine learning coupled with atomistic calculations for predicting properties in complex materials

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High entropy materials (HEMs) present a paradigm shift in materials design. A signature feature of HEMs is the presence of multiple principal elements in large proportions in contrast to one principal element in conventional/dilute alloys. Originally observed in high entropy alloys (HEAs), the concept has broadened to other materials classes including oxides, borides and nitrides. While these materials present opportunities to unravel novel properties due to a large compositional phase space, they also present an equally large challenge to survey the phase space and locate interesting compositions thereby presenting a data-science challenge. Additionally, the presence of multiple elements results in local lattice distortion (both atomic and electronic) thereby making the composition-property interface a very complex area. We present a machine learning coupled atomistics methodology whereby properties in complex materials could be predicted by learning from the database of simpler materials. Three materials properties, including stacking fault energies, point-defect formation and migration energies, and vibrational entropy are predicted to demonstrate the approach. A major benefit of the approach is that as the database of simpler materials grows, the self-learning algorithm gradually sharpens its predictive capability and continues to expand into newer material compositions thereby overcoming the challenge of the phase space enormity.

Jacob Barker

Table-top turbulence simulators and adaptive optics for intense USPLs

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Intense, ultrashort-pulse laser (USPL) beams have various potential applications in the diverse areas ranging from remote sensing to directed energy. Mitigation of the detrimental effects of optical turbulence on the long-range propagation of USPLs is the key to unleashing this potential, yet very limited experimental and analytical data on the effects of turbulence on USPL propagation are available. The major obstacle to conducting a comprehensive investigation is the scarcity of experimental facilities that would comprise an intense USPL source, a controlled propagation range, and an adequate turbulence simulator. Here, we report a preliminary investigation and plans for follow-up research aimed at two major goals: (i) to devise an array of static and dynamic, table-top turbulence simulators that would adequately represent l ong-range, volumetric turbulence conditions and would be resistant to optical damage by intense USPL pulses and (ii) to develop effective adaptive optics (AO) strategies for the mitigation of the detrimental effects of strong air turbulence on the controlled USPL delivery to remote targets.

POSTER ABSTRACTS

Brandon Chalifoux

Ultrafast Laser Stress Figuring of Fused Silica Mirrors

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Fabricating freeform mirrors relies on accurate optical figuring processes capable of arbitrarily modifying low-spatial f requency height without degrading higher-spatial frequency errors. We present a highly scalable process to accurately figure thin mirrors using stress generated by a focused ultrafast laser. We applied ultrafast laser stress figuring (ULSF) to four fused silica mirrors to correct them to <20 nm RMS over 28 Zernike terms without significantly affecting higher-frequency errors. The accuracy and throughput for ULSF is on par with existing figuring processes, but unlike existing processes, ULSF can be applied after mirror coatings. Our current research efforts focus on scaling ULSF to higher throughput and larger range while maintaining the excellent accuracy already demonstrated.

Jim Field

Biotransformation and Microbial Toxicity of 2,4-Dinitroanisole (DNAN)

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2,4-dinitroanisole (DNAN) is a replacement for conventional energetic compounds (i.e., explosives), such as TNT because it is more stable and safer to handle. Little is known about DNAN's environmental fate. DNAN released to the environment might threaten ecosystems and public health. The objective of this study was to investigate the microbial transformation of DNAN in soils and wastewater sludge and characterize the microbial toxicity of these transformation products. Biotransformation was fastest under anaerobic conditions. Microbes reduced the nitroaromatic compound, forming aromatic amines which underwent coupling reactions to form azo dimers. Microbial toxicity tests showed that DNAN was highly inhibitory to methanogens and Allivibrio fischeri (Microtox bioassay). DNAN was more toxic than its monomeric daughter products. However, dimers, characterized with LC-QToF-MS, were the main metabolites formed after extended incubation, and these dimer mixtures were more toxic than DNAN. However, subsequent aeration resulted in extensive polymerization and a decrease in toxicity. Globally, our results suggest that DNAN undergoes reductive biotransformation in anaerobic environments leading to the formation of aromatic amines as well as dimeric metabolites that are eventually detoxified through extensive polymerization upon air exposure. These insights will help develop bioremediation strategies for DNAN pollution.

POSTER ABSTRACTS

Florian Goeltl

Cu-exchanged SSZ-13 in the conversion of methane to methanol

Authors:
Florian Goeltl

Cu-exchanged zeolites are known to efficiently convert methane, the main component of natural gas, to methanol. However, as of today the functioning of these materials is still under debate. In this contribution, the conversion of methane to methanol over Cu-exchanged zeolite SSZ-13 is investigated using first-principles based modeling. At a theoretical level, phase diagrams are used to identify the most likely active sites under a variety of conditions, reaction pathways and various spectroscopic signals for the most stable sites are calculated. Finally, theoretically predicted quantities are compared to experimentally measured observables and excellent agreement is found. The research presented here shows how theoretical modeling can be used to understand the performance of Cu-exchanged SSZ-13 in the conversion of methane to methanol. In the future it will be interesting to see how these insights can be transferred to other zeolite structures.

Roberto Guzman

Design of Novel Adsorbents for Detection and Isolation of Low Molecular Weight Peptide Biomarkers for Early Detection of Cancer

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In this work, agarose based chromatographic media have been engineered and synthesized for the separation and isolation of low molecular weight peptides (e.g., cancer biomarkers) from complex biological fluids (e.g., serum, saliva, urine, sweat, tears cerebrospinal fluid). Immobilized metal affinity chromatography (IMAC) was incorporated in these platforms for the binding of targeted biomarkers. Polymers such as m-PEG were incorporated to restrict large proteins from binding and interfering with the targeted peptides. Angiotensin I and II were used as model biomarkers (small molecular weight peptides with 1.3 and 1.015 kDa respectably). A complete separation of both angiotensins was achieve from human serum with two specific designed ligands, iminodiacetic acid (IDA) and dipicolylamine (DPA), and different metal ions..Early detection of any disease provides the best prospect for good outcomes. In exploring disease detection, a biopsy, a surgical invasive procedure, a section of the body is removed (tissue or cells) and examined to determine the presence and stage of a disease. A cancer biopsy for example is analyzed for the presence of tumor cancers. Alternatively, a liquid biopsy, a less invasive approach could offer some advantages since it does not involve any surgical procedure. In a liquid biopsy, a biological fluid such as blood (serum or plasma), urine, saliva, etc., is analyzed for the presence of components indicative of the presence of specific illnesses.

POSTER ABSTRACTS

Roberto Guzman

Engineering of Medical Implants: The Design of Novel Wound Healing Patch Loaded with Anticancer Therapeutics

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In this work, the design of a novel wound healing patch was engineered and synthesized through surface modification of chitosan's amine groups. The wound healing patch was designed to be used as a therapeutic for skin cancer. Anticancer drug, 5-fluorouracil, was incorporated into the film to prove treatment and to act as a prophylactic to metastasis of skin carcinoma. Metals were incorporated to act as chelating center to reduce flux of drug while also providing an antimicrobial agents. Implants are medical devices composed of biopolymers that have a future of immense importance. These biopolymers can be tailor made for any biological process through functionalization which allows for numerous applications. One of the applications that can benefit most from biopolymers is the skin's wound healing process. In chronic wound healing, healing can be accelerated or enhanced by providing an environment enriched with the proper nutrients and permeability necessary for the process to succeed. One process in which the healing process is essential is with skin cancer. In skin cancer treatment, it is common to remove the lesion surgically which leads to this impertinent healing process. While this treatment is effective it leads to a large defect that does not heal uniformly while also increasing the chances of metastasis. In this work, a chitosan-based nanomaterial artificial medical implant was synthesized and engineered to encapsulate anticancer drugs (5-fluorouracil, a cancer therapeutic) and wound healing materials while controlling the release flux and also providing antimicrobial, antiseptic, and antitumor properties.

Roberto Guzman

Functional Nanoparticles as Magnetic Resonance Imaging Agents and other Optical Biomedical Applications

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Nanoparticles show unique properties as a function of the different materials composition. These can be used to develop novel biomedical and technological systems.
In this work, we synthesize core-shell nanocomposites using different materials such as silica, metal oxides (e.g., iron, titanium, tellurium, zinc), noble metals, gold, silver, palladium, platinum and quantum dots of different compositions for imaging and contrast agents.
Characterization performed with SEM/TEM imaging for nanoparticle morphology and size. For the optical properties, UV-vis spectroscopy has been used. Energy dispersive spectroscopy EDS has been used to verify the element availability. Core-shell nanocomposites were synthesized using magnetic-gold-Titania. The size and the morphology of the particles were determined using SEM/TEM = 100 nm. A broadening light absorption was demonstrated with UV-vis spectroscopy. Future work will be considering embedding quantum dots on Titania for optical biomedical applications.

POSTER ABSTRACTS

Kyle Hanquist

Simulation of complex phenomena experienced during hypersonic flight

Authors:
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Hypersonic aerothermodynamics involves complex phenomena that can be of multi-physics, multidisciplinary, and vastly different timescales. For example, the hypersonic flow field is very complex, which includes nonequilibrium, reactive flows (i.e., chemistry), energy transfer between molecular energy modes, turbulence, boundary layers, unsteadiness, and shocks. This flow field interacts with the vehicle surface requiring the need for thermal protection systems and physics such as fluid-structure interactions, gas surface interactions, and ablation. One primary intention of hypersonic platforms is for responsive Intelligence, Surveillance, and Reconnaissance. It is common for these types of missions to employ radio frequency and electro--optical/infrared sensors to collect information. These signals are sensitive to the flow field motivating a need for a detailed understanding of the hypersonic flow field. While high-fidelity aerothermodynamic models are essential in minimizing the costs of physical and ground-based testing, they are prohibitively expensive when used in a many-query setting such as optimization, design, or full-scale vehicle analysis. This motivates multi-fidelity approaches, where each model trades a certain amount of accuracy for computational efficiency. This poster presents ongoing research by the Computational Hypersonics and Nonequilibrium research group in these areas.

Marat Latypov

Structural materials informatics for advanced defense applications

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The emergence of machine learning and data sciences offered the potential of accelerated materials design and discovery, thereby shaping the field of ‘Materials Informatics’. Significant progress has been made in materials informatics of fundamental single-crystal properties of materials. Yet, it has been challenging to adopt materials informatics methods for predicting and screening in-service performance of structural polycrystalline materials relevant to numerous defense applications. In this poster presentation, we outline research activities of our group at UArizona in developing Structural Materials Informatics strategies to fill this gap. We integrate experimental data, theory, machine learning, and network science to predict performance of structural materials ranging from strength predictions to high strain-rate mechanical behavior and high-cycle fatigue of polycrystalline and multiphase alloys.

POSTER ABSTRACTS

Euan McLeod

Soft Nano-Photonic Systems Laboratory

Authors:
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Our lab studies the interaction of light with structures derived from nanoscale colloidal building blocks using a mixture of experiment, theory, and computation. Our research includes investigations into the fundamental optical properties of these materials, manipulation of nanoparticles using optical tweezers, assembly of nanostructured photonic metamaterials and superresolution devices, integration of nanophotonic and microphotonic systems, and sensing of nanoparticles and biomolecules using lensfree holographic microscopy. This research will enable better microscopes, smaller and lighter optical devices, and more sensitive biomedical sensors.

Qiong Nian

A novel ensemble learning potential to study carbon atomic physics in diamond

Authors:
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In recent years, nitrogen doping in nanosized diamonds (NDs) is under extensive study to create the important point defect, nitrogen vacancy (NV) color center. NV center contained NDs are currently considered as the basic units for quantum computers, quantum cryptography, and quantum sensors towards single cell/molecular monitoring. However, NV-NDs are extremely difficult to manufacture in current research due to limited computational modeling tools that can precisely and efficiently predict carbon atom interactions in diamond phase formation, nitrogen doping, and NV center generation processes. Conventional empirical atomic potentials can achieve efficient simulation but with sacrifice of accuracy. Recent deep neural network atomic potentials on basis of density functional theories (DFT), is often associated with many parameters that render a time-consuming training process. To break this tradeoff and pursue a compromised high calculation efficiency and precision, we propose a new machine learning interatomic potential based on ensemble learning. We aim to develop a transferable carbon-carbon interatomic potential, where the predicted atomic physics (e.g., elastic constant, cohesive energy, etc.) can be determined by a 'committee' consisting of 'members' representing different empirical and physics-based potentials (e.g., the Tersoff potential for carbon and among others).

Adam Printz

Addressing the Thermomechanical and Chemical Instability of Metal Halide Perovskites Through Scalable Approaches

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This poster highlights some of our research group's efforts to address the thermomechanical and chemical instability of solution-processable metal halide perovskite semiconductors. These approaches range a span of length scales from molecular to bulk film and are all inherently scalable. While metal halide perovskites are used as a test case, these strategies are inherently extendable to many other solution-processable systems.

You Qiang

Development of Advanced Radiation Nano-Detector Using Machine Learning Approach

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This proposed effort focuses on radiation effects of novel nanocluster films as sensor nanomaterials for developing an advanced real-time radiation monitoring system. It consists of low-activation sensor material preparation, development of a real-time data acquisition, real-time study of electrical resistivity of the sensor materials under ion irradiation, neutron irradiation study, and modeling and simulation of microstructures and properties by using of machine learning (ML) approach. Recently, our preliminary results on the Fe-Fe_3O_4 core-shell nanocluster thin-film (with size < 1 cm^2) in which metallic Fe particles are covered by an oxide shell shows exceptional promise to act as a sensor for real time (in < 1 min) monitoring of neutron flux. For example, we observed that the in-situ resistance of the film under 5.5 MeV Si^{2+} ion irradiation at room temperature and 200 0C exhibit a super-exponential decay (~80%) even under a very low dose of 0.001 dpa of ion irradiation. Such behavior is not observed when heated up to 800 ºC or exposed to in-situ electron irradiation indicating that neither electronic nor thermal processes can explain such behavior. There are no any commercial detectors that can have such high sensitivity. Although our experimental observations are truly exciting, we lack fundamental scientific understanding of intriguing property change of Fe/Fe_3O_4 system under irradiation. We plan to develop fundamental understanding about the phase stability at Fe/Fe_3O_4 interface using a ML guided computational and experimental approach. This proposed research directly supports the DEPSCoR mission on the development of advanced radiation sensor technology.

POSTER ABSTRACTS

Prasanna Thoguluva Rajendran

UArizona's CFDWARP

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CFDWARP is an in-house CFD code developed and updated at the Computational Plasma & Reactive flow laboratory headed by Prof. B. Parent at the University of Arizona. It has the unique capability of simulating non-neutral plasma sheaths in fully-coupled form with the quasi-neutral bulk fluid flow. The coupling between the sheaths and the bulk flow is critical to simulate accurately MHD forces in planetary entry, plasma-assisted combustion in scramjet combustors, and electron transpiration cooling in hypersonic waveriders. CFDWARP can also simulate accurately turbulent flows such as fuel-air mixing or recirculation regions in scramjet inlet either using RANS or ILES/DNS.

Kenan Song

Innovative Manufacturing for 1D, 2D and 3D Composites

Authors:
Kenan Song, Weiheng Xu, Sayli Jambhulkar, Dharneedar Ravichandran

Layer-structured composites have broad applications in structural systems, thermal insulation, microelectronics, optics, and biomedical devices. The design and assembly of layered structures containing polymer and particle materials have been challenging in sub-microscale. The bottleneck is the lack of appropriate manufacturing compatible with soft matter and nanomaterials. This research will demonstrate three examples in 1D, 2D and 3D structures containing polymer and nanoparticle layers for different applications.

The first example was the use of polymer-nanoparticle interphase design to achieve 1D fibers. As well known that polymer fibers of microscale with continuous nanoparticle distribution are difficult to process due to the stiffness mismatching between polymers and nanoparticles. This example will demonstrate unique fiber spinning that blends polymers and nanoparticles at different layers. The soft macromolecules and rigid particles will be stacked along the radial or the fiber axis for enhanced mechanical, electrical, and thermal properties. The unique material system of composite fibers were used as piezo- and chemi-resistive sensors.

The second example exhibited a thin composite film on compliant structures for thermoelectric generators (TEGs). The stacking of 2D films contained conjugating polymers in-situ polymerized at the presence of nanoparticles. During the processing, the polyaniline molecules were found to coat evenly on carbon nanotubes and led to high electrical conductivity, power factor, and enhanced mechanics. Thus, these compressed films were exhibited on compliant structures and used as wearable devices for human body heat collection. The generated electricity was for powering wearable sensors in detecting human movement and health conditions.

The third demonstration utilized layer-by-layer-based deposition techniques. Both additive manufacturing (e.g., 3D printing) and coating methods were used on the same processing platform. One dimensional carbon nanofibers (CNF) and 2D MXene particles were used as examples to be selectively deposited on polymer surfaces with pre-printed patterns. The control of the surface patterns and the nanoparticle assembly conditions (e.g., thermodynamic parameters, nanoparticle interactions, solid-liquid-air contact lines, etc.) led to selective deposition and preferential alignment of nanoparticles. As a result, the conductive paths on the substrate were developed to be anisotropic; following this characterization, the multi-functional sensitivity to strain, temperature, chemical liquids and volatile organic compounds (VOCs) were also displayed.

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POSTER ABSTRACTS

Jekan Thangavelautham

Advancing Space Robotic Technologies to Secure On-Orbit and Cislunar Space Assets

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The Space and Terrestrial Robotic Exploration (SpaceTREx) Laboratory seeks to advance the nation's space and planetary robotics capabilities to tackle current and future challenges in aerospace defense and civilian domains. Utilizing an agile, creative, and energetic workforce, the laboratory is developing end-to-end rapid response design capabilities to meet urgent needs. This includes innovative technologies for Space Domain Awareness (SDA), on-orbit servicing and traffic management, strategic Cislunar development, and post-disaster management. There is an urgent need to maintain US leadership in all these areas and maintain the security of vital space assets that support our modern way of life.
Our program is seeking to advance three significant areas in robotics: (1) Next-generation, extensible, and transformative modular robots for rapid response applications. (2) Machine-learning-based automated design and control of robots to achieve near-optimal system-level performance and robustness. (3) Swarm systems to tackle large scale construction tasks. Our robot systems derive inspiration or working principles from biology and over the years, our advances in robotics have led to systems exhibiting or exceeding human-competitive performance in large-scale reconnaissance, site preparation, construction, and logistics tasks. These space swarms can operate in distributed numbers and deter an adversary from invading, blockading, or destroying vital space assets. Furthermore, these capabilities may play a part in on-orbit assembly and maintenance of ever-larger space structures. Our current program will develop the building blocks for this proposed research. We plan to refine these technologies to produce breakthrough integrated capabilities that play to our institutional strengths in space exploration

Zheshen Zhang

Quantum Information and Materials Laboratory

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I will introduce the research carried out in the Quantum Information and Materials Laboratory, including quantum materials, devices, and systems of quantum information technologies, with applications in ultraprecise sensing, secure communication, computing, and machine learning.

POSTER ABSTRACTS

Houlong Zhuang

Nitrogen-vacancy center analogs in diamond-like compounds

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The Nitrogen-vacancy (NV) center in diamond plays important roles in emerging quantum technologies. Currently available methods to fabricate the NV center often involve complex processes such as N implantation. Furthermore, diamond phase has limited thermodynamic stability in high temperature due to its susceptibility of graphitization. In diamond-like compounds such as C3BN, introducing polar B-N bonds may enhance thermodynamic stability. Besides, creating a boron (B) vacancy immediately leads to an NV center analog. We use density functional theory to explore the potential of this NV center analog as a novel spin qubit for applications in quantum information processing. Our preliminary data show that the NV center analog in C3BN possesses many similar properties to the NV center in diamond including a wide band gap, weak spin-orbit coupling, an energetically stable negatively charged state, a highly localized spin density, a paramagnetic triplet ground state, and strong hyperfine interactions, which are the properties that make the NV center in diamond stand out as a suitable quantum bit (qubit). We also predict that the NV center analog in C3BN to exhibit two ZPL energies that correspond to longer wavelengths close to the ideal telecommunication band for quantum communications. C3BN studied here represents only one example of A3XY (A: group IV element; X/Y: group III/V elements) compounds. We will investigate the other compounds of this family to have similar NV center analogs with a wide range of functional properties, promising to be new hosts of qubits for quantum technology applications.