

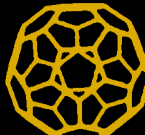


Materials @ Purdue Symposium

**2024 Final Program**

May 24th, 8am - 4pm

Forney Hall of Chemical Engineering

MSE  GSA

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## Materials @ Purdue Symposium (M@PS)

Thank you for attending Purdue's second interdisciplinary materials symposium! The Materials @ Purdue Symposium (M@PS) is a one-day event that highlights research from any material class done at Purdue. This event welcomes graduate students, post-docs, or undergraduates to present their completed or in-progress research. This symposium aims to celebrate the diversity of the field of materials within a multitude of departments at Purdue University. It also offers a platform for students to gain presentation experience, and for material researchers to learn about what other researchers are doing in our Purdue community.

## Materials Engineering Graduate Student Association (MSEGSA)

The Materials Engineering Graduate School Association (MSEGSA) is a group of materials engineering graduate students dedicated to promoting and improving the academic, social and professional well-being of the graduate students in the Purdue MSE department.

If you have any questions or feedback regarding M@PS or MSEGSA events, please contact [MSEGSA@purdue.edu](mailto:MSEGSA@purdue.edu)

## Useful Information

**Presentations** will be held at Forney Hall in room G124.

**Breakfast** will be catered from Great Harvest Bread Co, and additional **drinks** will be provided during breaks.

**Lunch** will be provided by Jimmy Johns, and lunchboxes will be reserved for those that have registered.

Please also note that there will be a strict "**no electronics**" policy for the duration of presentations.

The MSEGSA gratefully acknowledges funding from the College of Engineering for this event.

# Timetable

PO: Polymers, MX: MXenes, PV: Photovoltaics, E: Electronics, MT: Metals, C: Composites

## Presentation Itinerary

8:00–8:45	<b>Breakfast Catered by Great Harvest Bread Co</b>		
8:45–9:00	<b>Welcome remarks</b>		
9:00–9:15	PO	<b>Geeta Pokhrel</b> Chelsea Davis, John Howarter	Resilient Polymer Nanocomposites for Type II Thermal Interface Materials
9:15–9:30	PO	<b>Akul Seshadri</b> Reece Tippery, Liz Montagnino, Kendra Erk, John Howarter	Interactions of Silica-Functionalized Hydrogels with Cementitious Mixtures: Growth and Morphology of Inorganic Hydrates
9:30–9:45	PO	<b>Cindy L. Atancio-Martinez</b> Alexandre Lancelot, Jonathan J. Wilker	Formulation of Catechol-Containing Adhesives for Industrial-Scale Applications
9:45–10:00	<b>Break</b>		
10:00–10:15	MX	<b>Kat Nykiel</b> Alejandro Strachan, Babak Anasori	Exploration of Stacked MXenes as Precursors to Ultra-High Temperature Ceramics
10:15–10:30	MX	<b>Krutarth Kamath</b> Anupma Thakur, Nithin Chandran B S, Lia Stanciu, Babak Anasori	Time-Dependent Colloidal Stability of Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> MXenes Based on Ti <sub>3</sub> AlC <sub>2</sub> MAX Phase Purity, Synthesis Protocol, and Storage Conditions
10:30–10:45	MX	<b>Jacob Patenaude</b> Brian Wyatt, Kartik Nemani, Babak Anasori	Generalized Self-Assembly of Two-Dimensional Transitional Metal Carbides to Metal Powders
10:45–11:00	MX	<b>Annabelle Bedford</b> Anupma Thakur, Ornoba Chowdhury, Nithin Chandran, Maddie Lisenko, Bethany Wright, Brian Wyatt, Babak Anasori	High-Throughput Study of Rare Earth Doping in Double Transition Metal MAX and MXenes
11:00–11:15	<b>Break</b>		
11:15–11:30	E	<b>Samanvaya S. Gaur</b> Alexander V. Kildishev and Ernesto E. Marinero	Low-Damping Ferromagnetic Co <sub>1-x</sub> Fex Thin Films for Applications in Magnonics
11:30–11:45	E	<b>Karthika Haridas</b> Shubhra Bansal	Numerical Simulation of Superstrate CdTe-2D MoTe <sub>2</sub> Thin-Film Tandem Solar Cells
11:45–12:45	<b>Lunch Catered by Jimmy Johns</b>		

12:45–1:00	E	<b>Faharia Hasan Bhuiyan</b> Shubhra Bansal	Electromigration Lifetime of Fine Pitch Interconnects and Through-Silicon Vias for 3D-Heterogeneous Integration
1:00–1:15	E	<b>Md Habibur Rahman</b> Arun Mannodi-Kanakkithodi	Accelerating Defect Predictions in Semiconductors Using Graph Neural Networks
1:15–1:30	E	<b>Huilong Liu</b> Walter J. Smith, Maitreyo Biswas, Thomas Beechem, M. K. Arun Kumar, Shubhra Bansal	Dimensionally Modified Pt-Based Halide Perovskites
1:30–1:45	<b>Break</b>		
1:45–2:00	MT	<b>Poonchezhian Vishnu Prakash</b> Eshan Ganju, and Nikhilesh Chawla	X-Ray Microscopy Assisted 4D Analysis of Fatigue Crack Growth in Peened Gusset Plate Joints
2:00–2:15	C	<b>Adeline Ripberger</b> Yagmur Onder, Owen Plunkett, Colin Riley, and Jan-Anders Mansson	Feel and Control of Tennis Rackets: Inter- and Intra-Racket Correlations
2:15–2:30	C	<b>Alyson Pickering</b> Jan-Anders Mansson	Cost-Performance Relationship of Recycled Automotive Hybrid Molded Composites
2:30–2:45	C	<b>Seokkyoon Hong</b> Haozhe Zhang, Junsang Lee, Tianhao Yu, Seungse Cho, Taewoong Park, Julia Walsh, Yuhyun Ji, Joshua Jeremiah Kim, Hyowon Lee, Dong Rip Kim, Baoxing Xu, Chi Hwan Lee	Spongy Ag Foam for Soft and Stretchable Strain Gauges
2:45–3:00	<b>Concluding remarks</b>		

# List of Abstracts

## Oral Presentation Abstracts

### Resilient Polymer Nanocomposites for Type II Thermal Interface Materials

*Geeta Pokhrel, Chelsea Davis, John Howarter*

PO

School of Materials Engineering

Thermal interface materials (TIMs) in electronics are typically used between the heat source and heat sink to enhance heat dissipation. TIMs are continuously exposed to harsh conditions such as temperature cycling, mechanical stress, humidity, vibration, and shock, which can lead to failure and hinder efficient thermal conduction. Both thermal and mechanical properties are equally important for electronic reliability and performance. However, mechanical properties are often overlooked in the literature compared to thermal properties. This study emphasizes the fabrication of TIMs based on thermoplastic elastomer (TPE) nanocomposites with mechanical robustness and sufficient thermal conductivity. The form factor of the TIM is Type II, an elastomeric thermal pad. Mechanical robustness in the TIMs is achieved through triblock copolymers of polystyrene-block-polyisoprene-block-polystyrene (SIS). Thermal conductivity of these robust films is enhanced by incorporating functionalized 2D hexagonal boron nitride (BN) nanoplatelets. Mechanical behavior was analyzed using a uniaxial cyclic tension test at various (50%, 100%, and 150%) strains. In-plane thermal conductivity measurement was performed via Laser-based Angstrom method and cross-plane thermal conductivity via the Miniaturized Reference Bar Method. Above 20 vol.% BN, both in-plane and cross-plane thermal conductivities decrease. Additionally, the incorporation of the nanoplatelets increases surface roughness, elastic modulus, and mechanical hysteresis affecting residual deformation. We observe that an increase in nanofiller content above 20 vol.% negatively impacts mechanical performance without necessarily improving thermal conductivity. Thus, understanding the balance of mechanical and thermal performance is critical for optimization. The results obtained through this research can offer valuable insights for designing high-performance elastomeric thermal pads.

## Interactions of Silica-Functionalized Hydrogels with Cementitious Mixtures: Growth and Morphology of Inorganic Hydrates

*Akul Seshadri Reece Tippery, Liz Montagnino, Kendra Erk, John Howarter*

PO

School of Materials Engineering

Superabsorbant Polymer (SAP) hydrogels are crosslinked hydrophilic polymer networks that can hold and release several times their mass in water. This water transport behavior has been harnessed to internally cure cement. Recent work in our group is focused on functionalizing SAPs with organic silicate groups that allow the SAP to nucleate and grow cement strengthening phases. SAPs were formulated with nanosilica crosslinks through the incorporation of an organoalkoxysilane monomer 3-(trimethoxy silyl) propyl methacrylate (TPM). The resulting SAPs were shown to have dynamic swelling and dissolution behavior dependent on their TPM content through gravimetric swelling tests. Further SEM analysis showed morphological differences of SAPs in cured cement microstructures dependent on TPM content. Chemical composition of hydrate phases in SAP voids was investigated through Raman Microscopy and Energy Dispersive Spectra (EDS). To probe the origins of the morphological and chemical differences, Calcium Silicate Hydrate (C-S-H) was precipitated within SAPs through a double diffusion method. The inorganic growth, morphology, and interactions with the polymer network were studied through Small Angle X-Ray Scattering (SAXS). Chemical nature of the cementitious products within the SAP were investigated through Fourier Transform Infrared Spectroscopy (FTIR).

## Superabsorbent polymer hydrogels in sustainable cement applications

*Cindy L. Atancio-Martínez, Alexandre Lancelot, Jonathan J. Wilker*

PO

Department of Chemistry

Many catechol-containing biomimetic polymers inspired by marine mussels have been synthesized within the last decade. They have served as starting materials for the development of adhesives, hydrogels, coatings, and drug delivery systems, amongst others. With the increased popularity of catechol chemistry, it becomes essential to evaluate the potential production of such mussel-mimetic polymers at industrial scales. Here, we have scaled up the suspension copolymerization of poly(vinylcatechol-styrene) (PCS) to produce batches of 60g in an academic setting. The under water adhesion performance of PCS was studied and optimized to yield high strengths when dissolved in non-toxic and readily available solvents. Additionally, the concentration of PCS in solution was further investigated to produce an easy-to-apply adhesive in both dry and wet conditions. The bonding strength of PCS also showed superior performance when compared to commercial glues formulated for under water applications that utilize popular adhesive chemistries like epoxies, cyanoacrylates, and urethanes. Furthermore, the adhesive properties of our catechol-containing polymer exhibited promising results when tested on a variety of low- and high-energy substrates, as well as in lap shear and 90° peel fashions. Our novel and scalable synthetic approach, as well as the optimized formulation of catechol copolymers, brings us closer to introducing a new adhesive chemistry to markets.

# Exploration of Stacked MXenes as Precursors to Ultra-High Temperature Ceramics

*Kat Nykiel, Alejandro Strachan, Babak Anasori*

A circular logo with a yellow background and the letters 'MX' in black.

School of Materials Engineering

Ultra-high temperature ceramic (UHTC) zeta phases are critical for applications over 2000°C due to their high melting temperatures, oxidation resistance, and fracture toughness. However, the synthesis of zeta phase systems typically requires high temperature processing at >1400°C with high pressures, making alternative synthesis pathways to UHTC phases highly desirable. In this work, we investigate the potential of layered 2D MXenes as nanoceramic building blocks for nanolamellar carbide and nitride zeta-like phases. Stacked MXenes can expand the domain of zeta-like phases via their large space of interfacial combinations. We employed computational methods, primarily density functional theory (DFT), to investigate the thermodynamic stability of stacked MXenes as UHTC precursors, with sequential quasi-random structures to study non-stoichiometric nanolamellar carbides. We identify both stoichiometric and non-stoichiometric nanolamellar carbides below the established convex hull. Furthermore, we use a workflow that combines DFT simulations and machine learning to predict key UHTC features, such as melting temperature and elastic constants. Our findings show that by using stacked MXenes the UHTC domain can be expanded beyond vacancy-ordered zeta phases and traditional UHTC transition metals via a lower-temperature synthesis pathway.

# Time-Dependent Colloidal Stability of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXenes Based on Ti<sub>3</sub>AlC<sub>2</sub> MAX Phase Purity, Synthesis Protocol, and Storage Conditions

*Krutarth Kamath, Anupma Thakur, Nithin Chandran B S, Lia Stanciu, Babak Anasori*



School of Materials Engineering

MXenes, a family of two-dimensional transition metal carbides, nitrides, and carbonitrides, has expanded from the single composition Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> in 2011 to 50 compositions. Although nascent, MXene is taking center stage in 2D materials because of its exceptional properties owing to wide design and compositional tunability. Yet behind the spotlight lie numerous scientific challenges. One of the most pressing challenges is the chemical stability of MXenes. MXene flake-level defects, features, non-stoichiometry, and external stimuli contribute to susceptibility to attack by electron acceptors O<sub>2</sub> and H<sub>2</sub>O, leading to deterioration in ambient aqueous and atmospheric media. Negatively charged MXenes, albeit forming stable colloidal solutions in water, are highly prone to degradation by hydrolysis. In this work, we probe into relative scale of effects of a subset of stability determining factors for Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXenes, specifically Ti<sub>3</sub>AlC<sub>2</sub> phase purity, etching/delamination synthesis protocol, and storage conditions. For the Ti<sub>3</sub>AlC<sub>2</sub> precursor, we observed the difference between three kinds – non-stoichiometric oxycarbide (S-Ti<sub>3</sub>AlC<sub>2</sub>), optimized stoichiometric carbide (O-Ti<sub>3</sub>AlC<sub>2</sub>) and commercially available Sigma Aldrich Ti<sub>3</sub>AlC<sub>2</sub> (SA-Ti<sub>3</sub>AlC<sub>2</sub>). For the etching / delamination agents, we used two different routes – mixed acid MAc (HF + HCl with LiCl as an intercalant) and minimally intensive layer delamination MILD (LiF + HCl) method. Finally, to understand the effect of storage conditions we took into consideration the concentration (0.05 mg/ml and 1.0 mg/ml) and lighting condition (stored in a dark box and under constant light exposure in photobooth) of the stored Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> solutions.

# Generalized Self-Assembly of Two-Dimensional Transitional Metal Carbides to Metal Powders

*Jacob Patenaude, Brian Wyatt, Kartik Nemani, Babak Anasori*

MX

School of Materials Engineering

Two-dimensional (2D) transition metal carbides and nitrides, known as MXenes, are a family of nanomaterials with impressive material behaviors, such as their mechanical stiffness (386 GPa for Nb<sub>4</sub>C<sub>3</sub>T<sub>x</sub> MXene), electrical conductivity (up to 24,000 S•cm<sup>-1</sup> for Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>), electromagnetic shielding capability (up to 99% shielding efficiency at a 40-micron film for Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>), and hydrophilic surface groups (-40 mV zeta potential in water). MXene-metal composites are a field of growing interest for fields such as materials science, energy engineering, and mechanical engineering. For example, recent studies have demonstrated the self-assembly of MXene to Al powders to form scalable self-assembled powder mixtures suitable for mechanical reinforcement (40% improvement in Vickers Hardness for 2 wt.% Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> in Al). However, to further develop MXene-metal composites for manufacturing scales, we developed a generalized self-assembly process of 1 nm MXene flakes with a range of different metal powders (e.g. steel, titanium, niobium) using an acidic aqueous solution. Afterwards, we demonstrate the scalability of this process and illustrate its potential for manufacturing-scale powder beds for additive manufacturing of MXene-metal composites. We also show improvements in composite harness over steel alone (initial measurements showed a 10% increase in average hardness value). This presentation demonstrates the capability of MXenes for metal composites via a generalized, scalable self-assembly approach, tailored to additive manufacturing.

## High-Throughput Study of Rare Earth Doping in Double Transition Metal MAX and MXenes

*Annabelle Bedford, Anupma Thakur, Ornoba Chowdhury, Nithin Chandran, Maddie Lisenko, Bethany Wright, Brian Wyatt, Babak Anasori*

MX

School of Materials Engineering, \*Department of Chemistry

MXenes, two-dimensional (2D) transition metal carbides, nitrides, or carbonitrides, have grown rapidly as a nanomaterial family over the last decade for applications in energy storage, catalysis, electromagnetic interference (EMI) shielding, and beyond. The incorporation of rare-earth (RE) elements into MXenes can open a wide range of applications, from magnetic 2D materials for quantum computing and EMI shielding to electrocatalysis. However, until now, the instability of RE elements in the transition metal sites in previous studies during top-down etching has limited the synthesis of RE-containing MXene from their parent MAX phases. Recently, RE-doping in nanostructures ranging from semiconductors to inorganic-organic hybrids has resulted in tunable optical, electrical, magnetic, and catalytic properties. Here, we present a high-throughput synthesis study of a series of RE-doped MAX phases and their MXenes, using five MAX/MXene compositions with three RE dopants (Nd, Gd, Tb). This investigation involves systematically incrementing molar stoichiometric ratios of RE to transition metal elements in the MAX phases. To determine the RE-doping into the selected MAX phase, we used x-ray diffraction and scanning electron microscopy with energy dispersive x-ray spectroscopy. Afterward, the successful RE-doped MAX phases were etched to form MXenes. The selective etching and delamination experiments were tuned to minimize the harsh environmental effects, which could oxidize existing rare earth components. This high throughput study expands the available compositions of MXenes with the incorporation of RE, which may further explore 2D RE-MXenes in magnetic or quantum electronics.

# Low-Damping Ferromagnetic Co<sub>1-x</sub>Fe<sub>x</sub> Thin Films for Applications in Magnonics

*Samanvaya S. Gaur, Alexander V. Kildishev and Ernesto E. Marinero*

E

School of Materials Engineering

Progress in information processing technology is hindered by energy dissipation in the form of Joule losses that reduce the efficiency of data storage and transport. Potential alternatives include devices that operate by utilizing spin wave excitation and propagation (magnons) in magnetic materials. In such systems, low damping of spin wave excitations is a critical parameter to control the precessional motion of magnetization and it determines the propagation length of magnons. Thus far, conventional ferrimagnetic yttrium iron garnets (YIG) exhibit the lowest damping constant and are today's material of choice for magnon generation and transport (magnonics). However, the need for epitaxial growth of YIG on single crystal substrates of Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> at elevated temperatures (900°C) limits their scalability and their integration in devices employing CMOS fabrication processes. Alternatively, Co<sub>25</sub>Fe<sub>75</sub> is a promising candidate such that despite being a ferromagnet it exhibits low damping ( $10^{-3}$ ) and its significance is highlighted by the fact that it can be easily grown as a polycrystalline film by sputter deposition on SiO<sub>2</sub> at room temperature. In this presentation, I will present recent results from my study in which I fabricated a series of Co<sub>1-x</sub>Fe<sub>x</sub> alloys with % Co ranging from 23 % to 36 % (SiO<sub>2</sub>/Ta(3nm)/Cu(3nm)/Co<sub>1-x</sub>Fe<sub>x</sub>(10nm)/Cu(3nm)/Ta(3nm)). Interestingly, I obtained a new low in damping for Co<sub>25</sub>Fe<sub>75</sub>  $1.43 \times 10^{-3}$  and unexpectedly Co<sub>36</sub>Fe<sub>64</sub> exhibited the lowest damping of  $0.91 \times 10^{-3}$ . Overall, there is a decreasing trend in damping as the % Co increased this is attributed to better lattice matching with the Cu buffer layer. This lattice correlation will be explained in detail as well. Further, some interesting results from magneto-optic modeling will also be presented that show the potential of this ferromagnetic material to be implemented in nanoscale magnonic devices.

# Numerical Simulation of Superstrate CdTe-2D MoTe2 Thin-Film Tandem Solar Cells

*Karthika Haridas, Shubhra Bansal*



School of Materials Engineering

CdTe exhibits a direct bandgap of 1.45 eV with high absorption coefficient, however, efficiency of record devices is reported at 22.1%, significantly lower than the Shockley-Queisser detailed-balance limit. Record 16.5% devices in 2001 achieved open-circuit voltage ( $V_{oc}$ ) of 0.848 V, which has marginally increased to 0.887 V for state-of-art devices, only 72% of 1.23 V calculated based on detailed-balance approach. Even though the  $V_{oc}$  is limited in CdTe devices, recent advances in efficiency have resulted from improved photon transmission to CdTe layer, bandgap grading, novel contacts, and bifocality using electron reflectors. The efficiency of CdTe thin-film solar cells can be increased beyond single junction S-Q limit, with integration of a compatible low-bandgap bottom cell. In this study, we employ SCAPS-1D simulations to investigate the performance of CdS/CdTe top-cell with three low-bandgap ( $E_g = 1.1$  eV) bottom cell options, namely p-type 2D-MoTe2 compared with traditional thin-film photovoltaic materials such as p-Sb<sub>2</sub>Se<sub>3</sub> and p-CIGS (Copper Indium Gallium di-Selenide). The first objective was to evaluate the effect of addition of n-MoTe<sub>2</sub>/ p-type MoTe<sub>2</sub> bottom cell on the efficiency of CdS/CdTe single-junction cell. The second objective was to conduct a comparative analysis with p-type Sb<sub>2</sub>Se<sub>3</sub> and p-type CIGS as bottom cell absorbers on the efficiency and band alignment of the tandem solar cells. Initial simulation results reveal promising efficiencies for the p-type MoTe<sub>2</sub> - CdTe tandem solar cell around 42%, showcasing its potential as a viable photovoltaic technology. Design of 2- and 4-terminal tandem devices with 2D-p-MoTe<sub>2</sub> bottom cell technology will also be discussed.

# Electromigration Lifetime of Fine Pitch Interconnects and Through-Silicon Vias for 3D-Heterogeneous Integration

*Faharia Hasan Bhuiyan, Shubhra Bansal*

E

School of Materials Engineering

With the inception of “more than Moore” concept, there is a shift towards advanced packaging, wherein, chiplets can be heterogeneously integrated into a single package. As the advanced front-end node dimension evolves to sub-5 nm dimensions, advanced high-density packaging technology must be developed accordingly to address the signal transfer and heat dissipation issues. These requirements lead to aggressive scaling down of interconnects such as through-silicon vias (TSVs) and micro-bumps to sub-micron dimensions for applications such as high-bandwidth memory. At the same time, with increasing power density and heat dissipation requirements, subject these interconnects to high current density and temperature conditions, leading to failure mechanisms such as electro-, thermo- or stress- induced migration. Hence, an understanding of migration of atoms driven by electron wind, temperature and stress gradients is important to determine failures in advanced interconnects. Here, we evaluate the effect of interconnect aspect ratio, current density, and temperature on the electromigration lifetime, using a COMSOL Multiphysics model. Vacancy flux is estimated based on atomic flux due to electron wind, stress, temperature, and concentration gradient, with diffusion flux in the opposite direction as electron-wind flux. Additionally, we aim to investigate the effects of different types of barrier and capping layers on the electromigration resistance of Cu interconnects. Using the continuity equation, the normalized vacancy concentration, hydrostatic stress and Von-Mises stress distribution can be estimated as a function of time. A combination of experimental and numerical modeling can serve as a framework for materials selection and reliability prediction for fine-pitch interconnects.

# Accelerating Defect Predictions in Semiconductors Using Graph Neural Networks

*Md Habibur Rahman, Arun Mannodi-Kanakkithodi*

E

School of Materials Engineering

First-principles computations reliably predict the energetics of point defects in semiconductors but are constrained by the expense of using large supercells and advanced levels of theory. Machine learning models trained on computational data, especially ones that sufficiently encode defect coordination environments, can be used to accelerate defect predictions. Here, we develop a framework for the prediction and screening of native defects and functional impurities in a chemical space of group IV, III-V, and II-VI zinc blende semiconductors, powered by crystal Graph-based Neural Networks (GNNs) trained on high-throughput density functional theory (DFT) data. Using an innovative approach of sampling partially optimized defect configurations from DFT calculations, we generate one of the largest computational defect datasets to date, containing many types of vacancies, self-interstitials, anti-site substitutions, impurity interstitials and substitutions, as well as some defect complexes. We applied three types of established GNN techniques, namely crystal graph convolutional neural network, materials graph network, and Atomistic Line Graph Neural Network (ALIGNN), to rigorously train models for predicting defect formation energy (DFE) in multiple charge states and chemical potential conditions. We find that ALIGNN yields the best DFE predictions with root mean square errors around 0.3 eV, which represents a prediction accuracy of 98% given the range of values within the dataset, improving significantly on the state-of-the-art. We further show that GNN-based defective structure optimization can take us close to DFT-optimized geometries at a fraction of the cost of full DFT. The current models are based on the semi-local generalized gradient approximation-Perdew-Burke-Ernzerhof (PBE) functional but are highly promising because of the correlation of computed energetics and defect levels with higher levels of theory and experimental data, the accuracy and necessity of discovering novel metastable and low energy defect structures at the PBE level of theory before advanced methods could be applied, and the ability to train multi-fidelity models in the future with new data from non-local functionals. The DFT-GNN models enable prediction and screening across thousands of hypothetical defects based on both unoptimized and partially optimized defective structures, helping identify electronically active defects in technologically important semiconductors.

## Dimensionally Modified Pt-Based Halide Perovskites

*Huilong Liu, Walter J. Smith, Maitreyo Biswas, Thomas Beechem, Arun Mannodi-Kanakkithodi, Shubhra Bansal*

E

School of Materials Engineering

Platinum halide perovskites are intriguing and eco-friendly alternatives for the toxic lead-halide perovskites not only maintaining merits including solution processibility and remarkable optoelectronic properties, but also demonstrated with extraordinary stability. Dimensionality was affirmed to play a significant role in the properties of perovskite materials. Comparing to 3D halide perovskite in which the metal-halide octahedron connects three dimensionally in high symmetry, reducing the structural dimensionality to lower degree (2D or 0D) can generally lead to improvements in environmental stability, as well as influencing the bandgap, band dispersion, and exciton binding energy of the material due to formation of quantum wells (QWs) and quantum confinement effects. The phenomenon of the ISC and the singlet exciton-to-triplet exciton transfer has also been reported in many perovskite-acceptor complexes and 2D-perovskites (e.g. (MA)<sub>2</sub>Pb(SCN)<sub>2</sub>I<sub>2</sub>). Engineering the energy transfer from the perovskite to an acceptor dye in the form of a triplet (or singlet) state offers additional opportunities to tune the properties of the semiconductor–dye hybrid and its highly potential in the application of room temperature phosphorescence or triplet-triplet annihilate (TTA) up-conversion device/application. Herein, we were the first to propose the synthesis and characterization of the 2D Pt halide perovskite CsPtI<sub>3</sub>(DMSO), which exhibits unique characteristics (e.g., large shift between the absorption edge and PL emission due to singlet-triplet intersystem crossing (ISC) and phosphorescence) and significant potential in photovoltaic applications (e.g., Triplet-triplet annihilate (TTA) up-conversion). The solution-processed thin films (via blade coating) were characterized with various routine techniques including SEM, EDS, XRD, FTIR, UV-vis spectroscopy, PL/Raman, and TGA.

# X-Ray Microscopy Assisted 4D Analysis of Fatigue Crack Growth in Peened Gusset Plate Joints

Poonchezhian Vishnu Prakash, Eshan Ganju, Nikhilesh Chawla

MT

School of Materials Engineering

Gusset plates are essential for connecting beams, girders, columns, and other structural elements in bridges. These structures often face cyclic loading, leading to fatigue crack growth, particularly in welded areas. If left unchecked, this can lead to catastrophic failure. This study aims to systematically study how peening enhances the fatigue life of welded gusset joints used in bridges and other structural elements. To simulate the gusset plate joints, dog bone samples with cruciform-welded gusset plates in the center were manufactured using A572 structural steel. The samples underwent different peening treatments—shot-peening, needle-peening, and shot-peening with grit blasting. Stress-controlled fatigue tests were carried out to evaluate fatigue life, and the results were compared to unpeened samples. To study the critical crack growth at various levels of cyclic loading, interrupted fatigue experiments were also carried out for each peening condition with non-destructive X-ray microscopy to assess the evolution of cracks within the samples. Stress-strain hysteresis and secant modulus plots were constructed for the fatigue tests of each condition, and they were studied to quantify the onset and evolution of damage. The results showed that peened samples have a significantly enhanced fatigue life compared to unpeened samples and that crack initiation was impacted by the different peening processes to different extents. The results also showed that the failure in the peened samples happened away from the gusset plates in the gage region near the grips, whereas the failure happened along the weld toes of the gusset plates in the unpeened samples.

## Feel and Control of Tennis Rackets: Inter-and Intra-Racket Correlations

*Adeline Ripberger, Yagmur Onder, Owen Plunkett, Colin Riley, and Jan-Anders Mansson*



School of Aeronautics and Astronautics

Historically, tennis rackets had wood frames but advancements in material science led to lighter and stiffer composite frames yielding faster ball speeds and improved performance. Although the increased stiffness improves performance it has also been linked to the harsher vibrations associated with tennis elbow, a common injury. This work aims to establish new racket evaluation “feel and control” criteria beyond the more traditional metrics “weight and stiffness.”

We have defined two “feel parameters.” Shock ratio is a measure of the forces felt at the handle after ball impact. Nervousness is a measure of lingering vibrations immediately following impact until the settling time. The racket vibration is recorded using experimental modal analysis. An instrumented hammer is used to strike the racket which oscillates freely on elastic bands while an accelerometer records the acceleration at the handle. The signal is processed in a custom-built MATLAB graphical user interface which calculates the feel parameters, natural frequencies, and damping ratios.

Shock and nervousness were measured for ten different rackets enabling examination of correlations between racket properties and feel parameters. Results show that shock ratio and nervousness are positively correlated with stiffness. As expected, the increased stiffness contributes to higher nervousness. Parameters from multiple impact locations are visualized across the string-bed providing insights into racket sweet spots. Shock ratio increases away from the center of the racket; aligning with player descriptions of harsh vibrations on off-center hits. Our current investigation includes exploring methods to modify feel parameters allowing for enhanced performance and injury prevention.

# Cost-Performance Relationship of Recycled Automotive Hybrid Molded Composites

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As the United States anticipates the arrival of legislation addressing the environmental impact of automotive production, manufacturers are looking to include upwards of 20% recycled material in new vehicle programs. In automotive applications, hybrid molded composites are favorable as a continuous fiber reinforcing preform, will carry the load in an over-molded part providing increased mechanical properties crucial for the crash performance of these parts. However, using recycled polymeric material poses challenges due to its reduced mechanical performance and increased variability. Moreover, the cost of recycled material often surpasses that of virgin material despite its reduced performance, posing a pressing dilemma for manufacturers as they are tasked with incorporating recycled material into future vehicles.

To investigate the impact of using recycled hybrid-molded composite parts on mechanical performance and cost, a part is constructed using a preform comprising unidirectional glass fibers (GF) within a Polypropylene (PP) matrix, and over-molded with short GF reinforced PP. The mechanical performance of this test part is characterized through the analysis of stiffness, tensile strength, elongation until break, and fiber length distribution. The cost implications are quantified through technical cost modeling considering part fabrication (the layup of the preform and injection molding) as well as the recycling process (shredding, and compounding). A framework capable of estimating both the cost and properties of final parts, based on initial process inputs, was developed. This model enables the quantification and optimization of tradeoffs between cost and properties, offering insights for navigating the challenges of integrating recycled materials into automotive production.

## Cost-Performance Relationship of Recycled Automotive Hybrid Molded Composites

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Strain gauges, particularly vital for wearable sensing, demand exceptional stretchability, softness, sensitivity, selectivity, and linearity. They must navigate challenges like mechanical and electrical hysteresis, overshoot behavior, and sluggish response/recovery times. Yet, existing strain gauges struggle to fulfill all criteria simultaneously due to inherent trade-offs. We introduce a novel approach utilizing spongy Ag foam with highly porous structures fabricated via steam etching using a pressure rice cooker to address these challenges. The formation of the micropores is attributed to the massive penetration and evaporation of the pressurized water molecules to/from the prepolymer during the steam-etching process. The eco-friendly process completes the process rapidly, contrasting conventional methods like lithography, templating, and 3D printing, which entail complex processes, high costs, and hazardous solvents. This approach offers a simpler, cost-effective, and environmentally friendly solution. The resulting highly porous structures lead to the enhanced internal surface area, deformability, sensitivity, and stability—ideal for strain sensing. Remarkably, strain gauges produced through this method exhibit an unprecedented gauge factor exceeding 8,000 at strains surpassing 100%, effectively meeting all requirements without significant compromise. Our work entails systematic investigations uncovering the complex structure-property-performance relationship of spongy Ag foam, demonstrated through practical applications like human motion monitoring and human-robot interaction. These breakthroughs pave the way for highly sensitive and selective strain gauges, showing immediate applicability across a wide range of wearable sensing applications.