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ABSTRACT:

Multi-Scale Modeling and AI-Guided Development of Multifunctional Reduced Dimensional Material for Defense and Space Technologies

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This presentation will highlight pioneering, multidisciplinary convergent science research conducted at our institute, which integrates modeling, nanotechnology, and photonics for defense applications. By leveraging novel chemical synthesis and materials processing techniques, we create AI and multiscale modeling-guided, multifunctional reduced dimensional core-shell nanoparticles, 2-D materials, and their mixed heterostructures. These are designed for transformative applications in defense technology, including space electronics and ground-to-space photonic communications. Innovations in materials capable of self-repair, adaptation to changing conditions, and resistance to extreme temperatures, high pressures, and high-radiation environments are binge explored. Applications range from protective coatings for aerospace vehicles to resilient structural materials for critical infrastructure. Special emphasis has been placed on the development of multifunctional materials that combine photonic or electronic properties with shielding capabilities against ionizing radiation or electromagnetic interference (EMI), including elastomers, reduced-dimensionality materials, and lightweight structures for radiation hardening.

Our objectives include: 1. Self-powered photonics and electronics for space awareness, collision avoidance, upconversion-based friend-foe identification, sensing and tracking, protection against direct high energy, and metamaterials and metasurfaces for dual ground to space IR and intersatellite communication components. 2. Quantum communication and sensing, defect engineering for single photon emission, multiwavelength LIDAR, and quantum spin defects for magnetic field mapping. 3. Materials for extreme environments, high entropy ceramic materials, 2-D materials, self-healing coatings, radiation-tolerant materials, and hypersonic materials.

Our multidisciplinary team is preparing rare-earth-containing MAX phase and MXene materials and their heterostructures and mixtures with other 2D materials. Four routes to rare-earth incorporation are being developed and optimized: (1) intercalation of rare-earth elements into conventional titanium carbide and molybdenum carbide MXenes, (2) synthesis and exfoliation of rare-earth containing MAX phases in which the rare-earth elements occupy “M” sites in the MXene, (3) fabrication of large-area, high-quality MXenes by chemical vapor deposition (CVD), and (4) fabrication of nanocomposites of rare-earth containing nanostructures with MXenes.

Our complementary combined use of AI, modeling, and simulation explores the optical linear and nonlinear properties as well as phonon bands of MXenes for electromagnetic shielding, photon down conversion and THz transmission. We also compute Raman spectra in support of Raman spectroscopic characterization of the synthesized materials. We conduct THz transmission measurements for these 2D materials along with EMI shielding measurements a RF to microwave frequencies.
In collaboration with Michigan State University, we are studying radiation effects on emerging 2D materials as the synthesis techniques allow. Characterization of fundamental properties before and after exposure to designed combinations of energetic heavy ions will document the basic tolerance of these materials to radiation environments involving heavy-ion strikes.
We are testing nanocomposites with self-healing vitrimers for their self-repairing properties to make them reusable.
This talk will conclude with a discussion of new opportunities for research.

P. N. Prasad “Nanophotonics” John Wiley & Sons, (2004)