Molecularly engineered inorganic nanomaterials and interfaces for novel properties

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Engineering nanomaterials and their heterointerfaces with control over multiple properties is crucial for diverse applications in electronics and energy. The first part of my talk will discuss a new class of high figure-of-merit bulk thermoelectric materials relevant to solid-state refrigeration. I will show that bulk pellets and thin films comprised of dilutely-doped nanocrystals of pnictogen chalcogenides and oxides exhibit multifold higher figures of merit arising from a combination of nanostructuring and isovalent doping-induced alterations to defect-chemistry and electronic-structure, leading to low thermal conductivities, and simultaneously high electrical conductivities and Seebeck coefficients, respectively. Electron spectroscopy and theoretical calculations point to key mechanisms including doping-induced carrier concentration control, suppression of antisite defects, and multifold increases in the density of states effective mass. The second part of my talk will describe the use of molecular nanolayers to tailor chemical, mechanical, thermal and electronic properties of metal-ceramic and metal-thermoelectric interfaces germane to device metallization and packaging. I will demonstrate that introducing molecular nanolayers (e.g., organosilanes, thiols, organophosphonates) at inorganic metal-oxide and metal-thermoelectric interfaces can produce remarkable multifold enhancements in interfacial fracture energy during static and dynamic loading, and thermal and electronic transport. Electron and ion beam spectroscopy, and X-ray and electron diffraction show that the property enhancements are due to molecular nanolayer-induced alterations to the inorganic interface chemistry and structure. Key mechanisms include strong bonding, interfacial oxide scavenging, diffusion curtailment, and altered phase formation. I will illustrate that molecular nanolayers can trigger unusual interfacial phenomena (e.g., viscoelastic bandgaps), provide a new approach for studying interface fracture nanomechanics through macroexperiments, and enable the design of high-interface-fraction organic-inorganic nanocomposites wherein molecularly-induced interface properties *become* materials properties.

Select References: Sci. Rep. 12, 10788 (2022); Nature Comm 9, 5249(2018); ACS Appl. Mater. Interf. (2017); ACS Appl. Mater. Interf. 8, 4275 (2016); Adv. Mater. 28, 6436 (2016); Nature Mater. 12, 118 (2013); Nature Mater. 11, 233 (2012); Nano Lett. 12, 4523 (2012); Nano Lett. 11(10), 4337 (2011); ACS Nano 4, 5055 (2010); Nano Lett. 10, 4417-22 (2010); Nature 447, 299 (2007); Appl. Phys. Lett. 104, 053903 (2014); Adv. Mater. Interf. 1500186 (2015); J. Vac. Sci. Technol., A 33, 020605 (2015); Scripta Mater. 121, 42-44 (2016); Appl. Phys. Lett. 109, 173904 (2016).

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Professor Ramanath received his PhD from the University of Illinois at Urbana-Champaign in 1997. His PhD thesis work won him a Graduate Student Award from the Materials Research Society. After a brief stint in the electronics industry, he joined Rensselaer in 1998 as an assistant professor, was promoted as full professor in 2006, and was named John Tod Horton Chaired Professor in 2013. His research focuses on developing a fundamental understanding of structure-processing-property relationships in molecularly-tailored inorganic thin film and bulk nanomaterials and interfaces, and harnessing them for energy and electronics applications.

Ramanath has co-authored more than 175 journal articles (Google Scholar h-index 51, 10,800 citations), one book chapter, and holds 9 US patents. He has delivered more than 230 invited/plenary/keynote talks worldwide, and has organized several international symposia and workshops for MRS, AVS and TMS. He co-founded *ThermoAura Inc*, served as the Director of the NY State Center for Future Energy Systems and an Editor of IEEE Transactions on Nanotechnology (2003-15).

Ramanath is a polyglot whose *hobbies* include Indian classical music (live and TV performances in the US, Australia, and India), Indic culture, philosophy, chants and devotional hymns, cricket, multilingual puns, poetry, and teaching spoken Sanskrit.

Honors and Awards (select)

- Fellow of the Materials Research Society (2018)
- Fellow of the American Physical Society (2017), Senior member IEEE (2017).
- Fellow of the American Vacuum Society (2013)
- Friedrich Wilhelm Bessel Award, Alexander von Humboldt Foundation, Germany (2013).
- Brahm Prakash Visiting Professorship, IISc Bangalore, India (2013).
- Rensselaer Team Excellence Award (2013); Rensselaer Research Excellence Award (Senior professor 2012, Early-career professor 2002).
- Alexander von Humboldt Fellow (2004)
- Professor Bergman Young Scientist Award US-Israel Binational Science Foundation (2003)
- National Science Foundation CAREER award (2000), IBM Research Partnership Award (2000-2013)
- Materials Research Society Graduate Student Award for Outstanding Research (1996).

Visiting Appointments

- Visiting Guest Professor, Advanced Functional Materials Laboratory, Department of Physics, Chemistry and Biology, Linköping University, Sweden (2019-).
- Distinguished visiting professor, PSG Institute of Advanced Studies, Coimbatore, India (2017-2018)
- Visiting professor, RWTH, Materials Chemistry Department, Aachen University, Germany (2013-14)
- Brahm Prakash Chair Professor, IISc, Bangalore, India (2013), Visiting Professor (2006)
- Visiting professor, The Max-Planck-Institute for Solid State Research, Stuttgart, Germany (2004-5)
- Visiting professor, NIMS-ICYS/WPI, Tsukuba, Japan (2004, 2010)
- Visiting professor, University of Wollongong, Australia (2007)