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High-temperature elastic moduli: a tool for understanding chemical bonding in thermoelectric materials

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Measurements of elastic moduli are of fundamental value for detecting changes in structure and bonding in solids, and, in the context of thermoelectric materials, are useful for explaining trends in lattice thermal conductivity, □□L. However, experimental elastic constants of functional materials are relatively sparse in the literature, and temperature-dependent data is even less common. We aim to address this, one material system at a time, using a technique called resonant ultrasound spectroscopy. In this talk, I will discuss how compositional changes and phase transformations (e.g., order-disorder, martensitic transitions) impact elasticity, and therefor thermal transport. First, we show that vacancies in the planar MX honeycomb lattice of AMX Zintls lead to a decrease in sound velocity and a sharp increase in point defect scattering, thus reducing □L by nearly 80%. The second part of the talk will focus on the effects of a supersonic phase transition - fundamentally an order disorder transition - in the layered CuCrX2 (X = S, Se, T). Lastly, we explore the (GeSe)1−x−(AgBiSe2)x system, in which alloying transforms the structure from orthorhombic to rhombohedral to cubic rock-salt, with the latter being the thermodynamically stable at a high temperature across the entire compositional range. We found an anomalous increase in the elastic moduli upon the transition from the rhombohedral to the cubic rock salt structure. Density functional theory suggests that this stiffening is caused by the tendency of Ge to exhibit strongly expressed lone-pair orbitals, which switch from fully oriented in the rhombohedral phase to randomly oriented in the cubic phase. Supporting this argument, decreased Ge content, and thus weakened lone-pair expression, leads to a less pronounced stiffening at the phase transition. These examples underscore the critical role of high-temperature elastic moduli in unraveling the complex interplay between chemical bonding, structural transformations, and thermoelectric properties, offering insight into the design and optimization of new materials.

Bio: Alexandra Zevalkink received her B.S. in Materials Science and Engineering from Michigan Technological University in 2008 and her Ph.D. in the same discipline at the California Institute of Technology in 2014. After completing her Ph.D., she pursued postdoctoral research at NASA's Jet Propulsion Laboratory and at the Max Planck Institute for Chemical Physics of Solids in Dresden, Germany. She joined the Department of Chemical Engineering and Materials Science at Michigan State University in 2016, where she is currently an C. Robert and Kathryn M. Weir Endowed Associate Professor. Her research focus is on the relationship between the atomic structure and bonding in inorganic materials and the resulting elastic, thermal and electronic properties. Her group employs a diverse set of tools including in-situ elasticity measurements, high-pressure and high-temperature X-ray diffraction, and a suite of single crystal growth and powder metallurgy techniques.