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POS-28 3D-to-2D transition of phonon transport in nanomaterials: a first-principles analysis

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Quasi-2D materials are composed of stacks of atomically thin layers. While individual monolayers have unique thermal and electronic properties on their own, quasi-2D materials introduce an array of new characteristics, such as anisotropic transport properties and thickness-dependent properties, which have important applications in optoelectronics and thermoelectrics. Our group is particularly interested in observing how the phonon/thermal transport properties of these materials behave as they transition from 3D bulk materials (strong interlayer coupling) to 2D nanomaterials (weak interlayer coupling). In particular, we use first-principles calculations to predict phonon dispersions, scattering rates, and thermal conductivities as we vary the distance between subsequent layers. Our current focus is on Rhenium Disulfide (ReS2), which maintains much of its monolayer characteristics in bulk form due to exceptionally weak bonding between layers. Our calculations will provide a detailed understanding of the unique thermal transport properties of these novel quasi-2D materials and may serve to motivate future technological innovation.

Author: STRONGMAN, Patrick (Dalhousie University)

Co-author: MAASSEN, Jesse (Dalhousie University)

Presenter: STRONGMAN, Patrick (Dalhousie University)

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