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Tuning Terahertz Vibrations for Thermal Energy Management

Thursday 4 December 2025 16:40 (30 minutes)

Atomic vibrations on the terahertz (THz) scale play a central role in determining a material's optical, electronic, thermal, and mechanical properties. In particular, the coupling between vibrational dynamics and thermal transport or phase transitions offers opportunities to design materials for efficient energy conversion and storage.

This presentation will highlight recent work investigating THz vibrations in functional materials used for thermal energy management. Neutron spectroscopy measurements—conducted on the Pelican spectrometer at the Australian Centre for Neutron Scattering—will be presented, demonstrating the ability of neutrons to directly measure THz-scale atomic motions. Case studies will include nanoparticles, thermoelectrics, simple organic molecular solids, layered organic–inorganic perovskites, and spin-crossover complexes.

Across these diverse systems, a unifying theme emerges: tailoring vibrational dynamics enables control over thermal transport and phase-change behaviour. For example, nano-carbon doping can suppress or redirect phonon transport in thermoelectrics, enhancing energy conversion efficiency [1]. Similarly, understanding vibrational modes in sugar alcohols informs their potential use as phase-change and thermal storage materials [2].

By comparing results across multiple classes of materials, this presentation will demonstrate how THz-scale dynamics underpin both fundamental understanding and practical advances in thermal materials. Neutron spectroscopy is shown to be an essential tool for this task, providing insights that bridge atomistic physics and macroscopic energy applications.

[1] Stamper, C.; Cortie, D.; Nazrul-Islam, S. M. K.; Rahman, M. R.; Yu, D.; Yang, G.; Al-Mamun, A.; Wang, X.; Yue, Z. Phonon engineering in thermal materials with nano-carbon dopants. Applied Physics Reviews 2024, 11 (2).
[2] Matuszek, K.; Kar, M.; Pringle, J. M.; MacFarlane, D. R. Phase Change Materials for Renewable Energy Storage at Intermediate Temperatures. Chemical Reviews 2023, 123 (1), 491–514.

Author: STAMPER, Caleb (Monash University)

Co-authors: CORTIE, David; YU, Dehong (Australian Nuclear Science and Technology Organisation); Dr MASON, Jarad (Harvard University); Dr MATUSZEK, Karolina (Monash University); LEWIS, Roger

Presenter: STAMPER, Caleb (Monash University)

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