DEPARTMENT OF PHYSICS
THE UNIVERSITY OF HONG KONG

Physics Colloquium

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Transport Physics and Search for Novel Thermoelectric Materials: from conventional to unconventional

April 30, 2025 (Wednesday)

5:00 p.m.

MWT4, 1/F, Meng Wah Complex, Main Campus, HKU

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Abstract:
This talk summarizes our integrated theoretical-experimental research on thermoelectric(TE) transport and material design through hierarchical chemical bonding frameworks and ordered-disordered sublattice coexistence approaches, synergistically regulating electrical and thermal transport by balancing strong/weak chemical bonds and lattice order-disorder states. The core concept aligns with the "electron crystal-phonon glass" paradigm, proposing a strategy to overcome traditional thermoelectric design limitations. For cage-structured skutterudites, multiple-filling BaxLayYbzCoSb3 systems were developed, achieving record thermoelectric performance (ZT=1.7–1.8) via broad-frequency phonon scattering (thermal conductivity 0.5–0.7 W/mK) and optimized charge transport by multivalence combinations. Part-crystalline-part-liquid/part-amorphous (or Liquid-like) thermoelectrics with crystalline-liquid/amorphous hybrid substructures (e.g. Cu2Se, Ag2(S,Se)) were engineered within hierarchical chemical bonding frameworks, breaking crystallinity constraints to realize atomic-scale order-disorder equilibrium and novel architectures. Align with the part-crystalline principle, multicomponent high-entropy systems like (Cu,Ag)(In,Ga)(Se,Te)2 etc were developed through sublattice engineering and entropy-driven strategies, employing pseudocubic lattice designs to balance atomic disorder and electrical transport optimization, achieving ultralow thermal conductivity while maintaining high conductivity. In searching for unconventional metallic thermoelectrics, ordered-disordered sublattice modulation enabled transformation of metallic systems (e.g. Fe/Co-based off-stoichiometry HHs) into high-performance materials via localized magnetic moments and correlated electron behavior control, achieving breakthrough Seebeck coefficients and figures of merits. These works establish a methodology integrating chemical bond gradient design, sublattice entropy regulation, and dynamic phase transitions for novel materials discovery. Current research advances frontier exploration in sublattice topological design and extreme-condition stability optimization, redefining material systems and performance boundaries beyond conventional semiconductor-based thermoelectrics.

Biography:
Dr. Wenqing ZHANG is Professor in Physics and Materials Science in Southern University of science and engineering. Prof. Zhang's research interests cover energy conversion and storage materials including thermoelectrics, catalysis and Li battery materials, computational materials science, machine learning and AI-aided materials design. Dr. Zhang was an elected APS Fellow due to his pioneering work in thermoelectric material design and computational materials science in 2013. He also serves as an APL editor for many years.

Anyone interested is welcome to attend.

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