Physics Colloquium

Tuesday, May 8th, at 3:30 pm in SC 234

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Unpacking structure-property relationships in thermoelectric clathrates

Inorganic clathrates are open-structured materials characterized by covalently bonded frameworks based on silicon, germanium, and tin, typically formed by face-sharing polyhedral cages that are large enough to encapsulate a variety of guest atoms inside. More than 20 years after Glen Slack's suggestion [1] and the subsequent discovery [2] that semiconducting variants might make good thermoelectric materials, clathrates remain the object of much experimental and theoretical study [3]. At the focus of many of these investigations is unraveling the microscopic mechanisms at the root of universally low and, in some cases, literally glass-like lattice thermal conductivities found in clathrates, that occur despite their apparently well-defined crystalline structure. In this talk, we will look at current thinking on thermal transport in intermetallic and inorganic clathrates, the influence of the guest atoms on the lattice dynamics, and how our understanding of these aspects has evolved with time. By highlighting recent insights gained from cutting edge experimental and theoretical studies, collective analysis of the available data, and persisting open questions, we will see how this unusual class of materials continues to push our understanding of the relationships between structure and thermal transport in crystalline materials, as well as our experimental and theoretical tools for studying these relationships.

[1] G. A. Slack, Mater. Res. Soc. Symp. Proc. 478, 47 (1997).
[2] G. S. Nolas, J. L. Cohn, G. A. Slack, S. B. Schujmann, Appl. Phys. Lett. 73, 178 (1998).
[3] M. Beekman, D. Morelli, G. S. Nolas, Nature Mater. 14, 1182 (2015).

Refreshments at 3:00 pm in SC 103