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Atomic structure vs. record-breaking performance: from magnetic to thermoelectric alloys

For an alloy theorist, “nature vs. nurture” boils down to “mean-field vs. structure”. Top-performance alloys are rarely random, and predicting a realistic atomic structure is as important as analyzing the resulting properties. The talk will start with a review of the state-of-the-art methodologies for making structural predictions, focusing on the techniques involving first-principles cluster expansion. It is possible to identify yet-unobserved low- T ordered phases even in widely used alloys, e.g. in Fe-Ni, Fe-Pd, and Fe-Pt. The ability to wisely navigate the chemical configuration space allows one to further endeavor onto optimizing specific alloy properties, such as seeking the specific atomic arrangements that maximize the Curie temperature of GaMnAs magnetic semiconductor.

The second part of the talk will illustrate how the knowledge of the atomic structure is used for analysis of superb thermoelectric performance in cubic telluride thermoelectrics. We first establish the miscibility limits and the atomic ordering (debated experimentally due to the small x-ray scattering contrast) in Pb-Ag-Sb-Te (LAST), one of the best-performing thermoelectric alloys. Further analysis predicts that pure AgSbTe₂ compound develops both a chemical and a dynamical instabilities, resulting in a strong off-stoichiometry, large Grüneisen parameter, and a low thermal conductivity, all observed experimentally. The electronic transport in AgSbTe₂ is found to require going beyond the approximations used in previous first-principles studies of thermoelectricity. Putting the pieces together, we arrive at a self-contained computational machinery for predicting both structural and transport materials properties.

**Wednesday, August 10, 2011
3:30 pm - Room 151, Jorgensen Hall**

Host:
Dr. Kirill Belashchenko
Department of
Physics & Astronomy

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