



# 复旦大学物理系物质科学报告

## Physics Department Colloquium

### Discovery of New and Old Thermoelectrics using First Principles

#### Methods

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Thermoelectrics are solid state energy conversion materials. They can be used to produce electrical power from temperature differences and can also be used for solid state refrigerators. They have been widely used in for spacecraft power as well as a number of niche applications. There is increasing interest in thermoelectric materials motivated in part by recent progress and in part by the potential of these materials in various energy technologies. Thermoelectric performance is a multiply contra-indicated property of matter. For example, it requires (1) high thermopower and high electrical conductivity, (2) high electrical conductivity and low thermal conductivity and (3) low thermal conductivity and high melting point. The keys to progress are finding an optimal balance and finding ways of using complex electronic and phononic structures to avoid the counter-indications mentioned above. In this talk, I discuss some of the issues involved in the context of recent results. One key aspect is optimization of the doping level in a given thermoelectric material. While this has long been understood in terms of standard semiconductor parabolic band models, we find surprisingly different results for many thermoelectric materials when the actual first principles band structures are used. This has led to prediction of a number of useful thermoelectrics, some that are new, and surprisingly some that are old.

**Time: 2:00 pm, Tuesday, 2014.01.07**

**Location: Physics Building, Room 221B**

(Cookies and coffee are served from 1:30 pm)