SEMINAR סמינר

A first-principles study of the role of substitutional elements in PbTe - based thermoelectric compounds for renewable energy applications

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The thermoelectric (TE) effect is manifested by direct conversion of heat flux into electrical power and vice-versa, and is utilized for power generation, waste heat recovery, and refrigeration. To optimize the power generation efficiency of a TE material, we require high values of Seebeck coefficient, which is the ratio of open-circuit voltage to the temperature difference across the TE element. Also, combination of high electrical conductivity with low thermal conductivity values is demanded to produce high electrical power, maintaining a relatively large temperature gradient across the TE device.

This study focuses on lead-telluride (PbTe), which is a promising TE compound employed for power generation at the mid-temperature range. Our goal is to optimize the chemical composition of PbTe by introducing substitutional point defects, to improve TE performance. To this end, we perform ab-initio calculations for PbTe-based compounds, based on the density functional theory (DFT). Our approach combines calculations of both vibrational and electronic properties, as follows. We derive the lattices' sound velocity and heat capacity from the elastic moduli, which are determined from total-energy calculations. Electronic transport properties are calculated applying the Boltzmann transport theory.

We test several substitution element; e.g., we find that electrical conductivity increases from 2.71×10^{4} to 3×10^{5} S m^{-1} at 700 K due to 6.3 at. % lanthanum doping, since La acts as electron donor. This trend is accompanied by monotonous reduction of thermal conductivity due to La-doping. Quantitatively, the average sound velocity decrease from 1980 m s^{-1} for the pure PbTe-lattice to 1347 m s^{-1} for the La-doped PbTe lattice, thereby reducing lattice thermal conductivity by ca. 32% at 700 K. As a general trend, we find that dopants belonging to the 4^{th}-5^{th} columns of the periodic table are the most effective in reducing lattice thermal conductivity, whereas dopants of groups 2, 14, and 16 are the most effective ones in increasing the power factor.

We, finally, demonstrate how this methodology could be generalized for dopant selection in other materials as well, oriented toward improving TE performance.

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ההרצאה תתקיים ביום ראשון, ה- 04 בינואר 2015 בשעה 14:30

באודיטוריום ע"ש דיוויד וואנג , קומה 3, בנין דליה מידן

The lecture will take place on Sunday, January 4th, 2015 at 14:30,

David Wang Auditorium, 3rd floor, Dalia Maydan Bldg.

כיבוד קל יוגש לאחר הסמינר