Philippe Jund, J Nanomed Nanotechnol 2013, 4:6
http://dx.doi.org/10.4172/2157-7439.S1.013

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference on
Nanotek & Expo

December 02-04, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

First principles study of nanostructured thermoelectric materials

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In the search of new sustainable energies, thermogeneration of electricity is one of the promising ways, notably because it is able to produce electricity from different kinds of heat wastes and to its portability. However, despite recent progress in the field, the state-of-the art materials have specificities making their mass-production difficult or even impossible: toxicity (thallium, chalcogen based alloys), weak abundance (tellurium based alloys) or cost (germanium or rare-earth based alloys). For all these reasons, finding thermoelectric materials without these drawbacks is vital if we wish to use thermoelectricity for generating electricity in the near future.

The talk will present a state-of-the-start numerical study of the properties of magnesium silicides which are promising materials in the high temperature range (T > 600K). In particular with the use of *ab initio* molecular dynamics simulations, how this type of approach can predict the stability (or not) of nanoclusters in the Mg2Si matrix will be shown. Indeed it has been shown that the use of nanostructured materials is of primary importance for a significant reduction in the thermal conductivity of the materials. This reduction has a positive impact on the thermoelectric coefficient of performance which will be described in the presentation.

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