**First-principles study of anomalous Nernst effect in Fe3Al and related compounds**

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The anomalous Nernst effect (ANE) has expected as a new mechanism of thermoelectric generation systems[1].The ANE magnitude can be enhanced either by two components as follows: (i) strong asymmetry of the anomalous Hall conductivity (AHC) along the energy axis; (ii) large product of Seebeck coefficient and Hall angle ratio[2]. The intrinsic contribution of AHC is induced by spontaneous magnetization[3]. It implies that large ANE could be found in magnetic materials with large anomalous Hall effect and/or large Seebeck effect.

Heusler compounds are one candidate materials to realize large ANE according to the two terms (i) and (ii)[4]. D03-type Heusler alloys Fe3Al is known as the ferromagnetic materials with Curie temperature of 760 K[5]. Furthermore, Fe2VAl in which one Fe atom of Fe3Al is substituted by V atom, which is correspond to 2 hole-doped per formula unit shows semiconductorlike behavior and large Seebeck coefficient (S=-180 µV/K) at room temperature[6].

In this work, we investigated carrier concentration dpendence of thermoelectric properties on Fe3Al and related compounds Fe2MnAl, and Fe2CrAl. We have performed first-principles calculations on Heusler compounds with OpenMX code[7]. The transport properties has been calculated based on the semiclassical Boltzmann transport theory with Wannier90 code[8]. We have found that a large ANE in hole-doped Fe3Al by using the rigid band apprximation. In the presentation, we discuss the origin of large ANE based on the systematic computations of thermoelectric properties.

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