Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

**Computational Discovery of New Heusler Compounds: Structures, Stabilities, and Applications** JIANGANG HE, VINAY HEGDE, CHRIS WOLVERTON, Department of Materials Science and Engineering, Northwestern University — Since their discovery by Fritz Heusler in 1903, Heusler compounds, $X_2YZ$, have been attracting a lot of research attention and have been intensely studied for their potential usage in spintronics, shape-memory devices, superconductors, thermoelectrics, topological insulators, and other applications. However, although more than 1000 Heusler compounds have been reported experimentally or computationally, a lot of potential Heusler compounds have not been explored yet due to complexities involved in dealing with such a huge phase space. As searching for new compounds experimentally is an expensive and a lengthy process, in this talk, we will demonstrate how to use a multi-step high-throughput computational screening method to predict several hundreds new stable and metastable Heusler compounds from 186588 compositions. As an example application, we will illustrate how to find age hardening precipitates using our screening strategy

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Date submitted: 06 Nov 2015 Electronic form version 1.4