# MM 15: Invited Talk: C. Scheu

Time: Wednesday 9:30–10:00 Location: H10

**Invited Talk** MM 15.1 Wed 9:30 H10

**Grain Boundary Defect Phases in Thermoelectric Materials: Impact on physical properties** — •Christina Scheu[1], Ruben Bueno Villoro[1], Siyuan Zhang[1], Baptiste Gault[1], Duncan Zavanelli[2], and Gerald Jeffrey Snyder[2] — [1]Max-Planck-Institute for Sustainable Materials, Max-Planck-Str. 1, 40627 Düsseldorf, Germany — [2]Northwestern University, Clark Street 633, 60208, Evanston, USA

Grain boundary defect phases are known since more than three decades, but mostly the impact on mechanical properties was investigated. In our work we were able to correlate the atomic structure and chemical composition of grain boundary defect phases in different thermoelectric materials to the electrical and thermal properties. For example, we were able to show by atom probe tomography and scanning transmission electron microscopy that grain boundaries in p-type Ti(Co,Fe)Sb Half-Heusler thermoelectric materials possess a significant Fe segregation and Co depletion compared to the bulk. Atomic column resolved scanning transmission electron microscopy images reveal that the grain boundary phase has a hexagonal close packed stacking compared to the face centered cubic stacking of the bulk with lattice distances differing from those of any known bulk phase. The grain boundary defect phase acts as fast charge carrier pathway providing a high electrical conductivity while simultaneously reducing the thermal conduc