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# From superconductivity towards thermoelectricity: Germanium based skutterudites

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Cage-forming compounds such as clathrates or skutterudites have proven to be not only of scientific but also of significant technological interest. The ability of these materials to accommodate guest filler species provides a wide range of varying physical and chemical properties. In skutterudites, the majority of cage forming elements is essentially based on volatile and/or toxic pnictogens like P, As and Sb. Recently, skutterudites $MPt_4Ge_{12}$ (M = Ba, Sr, La, Pr, Eu, Th, U) [1,2,3] have been discovered as the first members of a new class of skutterudites, based on a framework, entirely formed by Ge-atoms. These ternary compounds are well behaving metals and the majority of them are superconductors with transition temperatures below 10 K.

The aim of the present work is to demonstrate that a partial substitution of Ge by Sb modifies the metallic state leaving behind a metal with a substantially reduced charge carrier density. This is clearly demonstrated from first principle DFT calculations revealing a shift of the Fermi energy towards a gap in the electronic density of states. Accordingly, transport properties change and appreciably large improvements of the Seebeck coefficient are observed for $LaPt_4Ge_7Sb_5$.

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