High throughput screening of stability and thermoelectric properties in the transition metal silicides

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The phase stability, electronic structure and transport properties of binary 3d, 4d and 5d transition metal silicides are investigated using highthroughput density functional calculations. An overall good agreement is found between the calculated 0 K phase diagrams and experiment. We introduce descriptors for the phase-stability and thermoelectric properties and hereby identify several candidates with potential for thermoelectric applications. This includes known thermoelectrics like Mn_4Si_7, β-$FeSi_2$, Ru_2Si_3 and $CrSi_2$ as well as new potentially meta-stable materials like Rh_3Si_5, Fe_2Si_3 and an orthorhombic $CrSi_2$ phase. Analysis of the electronic structure shows that the gap formation in most of the semiconducting transition metal silicides can be understood with simple hybridization models. The observed trends in the structural stability are analysed in terms of a simple tight-binding model.