# Up- and Down Conversion of Functional (M-A-Ch) Materials - a strategy combining solid state synthesis of functional materials, resource efficiency and computational modeling

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In recent years we studied intensively ternary compounds in the phase diagram M-A-Ch with transition metal atoms M = Co, Ni, Rh, Pd, Ir, Pt; main group metals A = In, Sn, Tl, Pb, Bi, and chalcogen atoms Ch = S, Se, Te. Within the M-A-Ch phase diagram we identified the existence of different compositions along the line ACh + M: (i) $M_3A_2Ch_2$ type compounds can be deduced from antiperovskite structures when only half of M sites are occupied. Therein, $Co_3Sn_2S_2$ became famous as half metal and topological semi metal. [1, 2] For compositions $M_3A_2Ch_2$ a surprising variety of structures and compositions is found including layered shandite ($Ni_3Pb_2S_2$) type, monoclinic and superconducting parkerite ($Ni_3Bi_2S_2$) type structures, orthorhombic laflammeite and cubic $Pd_3Bi_2S_2$ that is a topological metal.[2] As further compositions (ii) skutterudite type $M_2A_3Ch_3$ compositions are found like $Ir_2Sn_3Te_3$ [3] besides of pyrite related compositions MACh for e.g. NiBiSe or PtSnS.[4] To understand the formation of competing compositions and structures reaction paths were studied from synthesis under high temperature and mild conditions from conversion reactions M + ACh. Further, we performed DFT-calculations to predict energy landscapes.[4] Studies on $Ni_3Sn_2S_2$ have shown, that different products like core-shell Ni@SnS, $Ni_3S_2$, Ni3Sn2 or SnS can be obtained by variation of reaction conditions (temperature, time, pH).[5] Further, for the examples of $Ni_3Bi_2Se_2$ and NiBiSe as well as for $Ir_2Sn_3Te_3$ and IrSnTe we could direct the reaction towards the formation of one of the target products.[6] We conclude that by modifying reaction conditions we can direct reactions to different products and even back to educts.

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