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Chemical bonding in layered thermoelectric materials Prof. Bo Brummerstedt IVERSEN

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Abstract: Layered (2D) materials exhibit a variety of extraordinary properties, and recent focus has included topological insulators, electrode materials, monolayers, hetero structures – and thermoelectrics. The physical properties such as band gap or thermal and electrical conductivity are related to the detailed structural characteristics as well as the specific chemical bonding both within the covalent layers and across the van der Waal gap. It is generally assumed that layered materials exhibit strongly anisotropic properties, but the properties are rarely discussed in direct relation to the specific chemical bonding characteristics of the solid.

Using advanced crystallographic analysis including charge density modelling as well as ab initio theoretical calculations we have studied the crystal structures and chemical bonding of a range of important layered thermoelectric materials including Cu_2Se , Mg_3Sb_2 , SnS_2 and TiS_2 .

