Layered Compounds: from Modular Description to Rational Design

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As a reliable *ab-initio* theory for crystal structure is still lacking, the rational design of new compounds remains a major challenge in solid state sciences. In that quest, the modular description of 2D structures could provide an interesting alternative pathway, as exemplified by the family of 2D-misfit layered chalcogenides $[(MX)_m]_{1+x}[TX_2]_n$ (M = rare earth, Sn, Pb, Sb or Bi ; T = Ti, V, Cr, Nb, or Ta ; X = S, Se) [1]. These compounds have incommensurate layered composite structures which are built from an alternated stacking of $[MX]$ module of the rock salt type and $[TX_2]$ module of the CdI_2 or NbS_2 types. Combinations of divalent or trivalent metals M and transition metals T led to the recognition of numerous new compounds with different alternated stacking sequences as defined by the m/n ratio. A careful analysis of structure databases proves that similar 2D modules (rock salt or CdI_2 types) are encountered in many structures and in many different chemical environments. This observation led to consider these modules as 2D building blocks and suggests a novel way to predict the structures and the compositions of some new inorganic compounds [2]. Starting from the modular description of misfit layered compounds this presentation aims to give an insight of the concept of 2D building blocks and to present its first application to the design of commensurate or incommensurate 2D layered compounds.

[1] *Materials Science Forum*, Trans. Tech. Publications, ed. by Meerschaut A., 1992, 100-101. [2] Cario L., Kabbour H., Meerschaut A., *Chem. Mater.,* 2005, **17**, 234.

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