

Why crystalize in layers: Chemical design principles for layered nonlinear optical crystals and topological materials

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The defining structural feature of all layered materials is distinct atomic layers held together by weak interlayer adhesion. It is not easy to rationalize why they adopt layered structures: e.g. why is MoS_2 layered rather than a fluorite, pyrite, or rutile structure, all with the same AB_2 stoichiometry. Here, we take the vantage point of two material families – each with competing 2D layered and 3D bulk phases – to rationalize the stability of their layered phases, based on principles in solid state chemistry and aided by free energy calculations at the density functional theory level. For the case of sylvanites, we show that 2D layered phases are intimately related to an ordered vacancy 3D bulk phase and can be stabilized at finite temperatures by vibrational entropy, similar to the well-known favorability of h-BN over c-BN at finite temperatures. Potential extensions to the relation between ordered vacancy carbides and MXenes are discussed. For the case of telluride compounds, we discuss an empirical rule rationalizing the layered structures of Bi_2Te_3 and MnBi_2Te_4 as a product of Peierls distortion. We then apply the same rule to predict new intrinsic magnetic topological insulators, followed by careful verification using first-principles theory. Overall, the chemical principles established in the two cases provide a means to rationally design and engineering layered functional materials.