Data Mining for More Than a Thousand Layered Materials, Hundreds of One-dimensional Materials and Lattice-commensurate Heterostructures

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Layered materials held together by weak interactions including van der Waals forces, such as graphite, have attracted interest for both technological applications and fundamental physics in their layered form and as an isolated single-layer. Only a few dozen single-layer van der Waals solids have been subject to considerable research focus, although there are likely to be many more and which could have superior properties. To identify a broad spectrum of layered materials, we present a novel data mining algorithm that determines the dimensionality of weakly bonded subcomponents based on the atomic positions of bulk, 3D crystal structures. By applying this algorithm to the Materials Project[2] database of over 50,000 inorganic crystals, we identify 1173 two-dimensional layered materials and 487 materials that consist of weakly bonded one-dimensional molecular chains. This is an order of magnitude increase in the number of identified materials, with most materials not known as two- or one-dimensional materials. Moreover, we discover 98 weakly bonded heterostructures of two-dimensional and one-dimensional subcomponents that are found within bulk materials, opening new possibilities for much-studied assembly of van der Waals heterostructures. [1]

Chemical families of materials, band gaps and point groups for the materials identified in this work are presented. Point group and piezoelectricity in layered materials are also evaluated in single-layer forms. 325 of these materials are expected to have piezoelectric monolayers with a variety of forms of the piezoelectric tensor. This work significantly extends the scope of potential low-dimensional weakly bonded solids to be investigated.

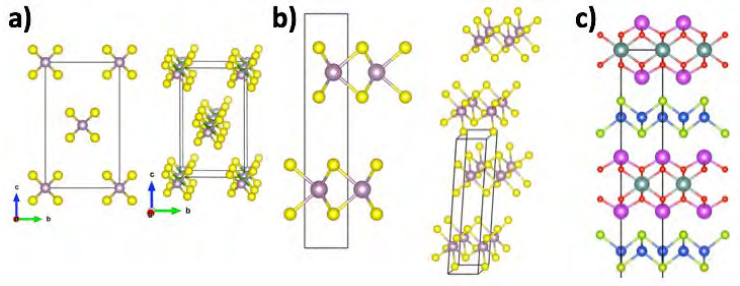

Figure 1 a), b): projection view(left) and perspective view(right) of example 1D and 2D weakly bonded solids. The atoms form one-dimensional chains in a), and two-dimensional planes in b). c): lattice-commensurate heterostructures with dissimilar layers, as opposed to the materials with same layers as in b).

[1] Cheon, G.; Duerloo, K.-A. N.; Sendek, A. D.; Porter, C.; Chen, Y.; Reed, E. J. Nano Lett. 2017.
[2] Jain, A.; Ong, S. P.; Hautier, G.; Chen, W.; Richards, W. D.; Dacek, S.; Cholia, S.; Gunter, D.; Skinner, D.; Ceder, G.; Persson, K. A. APL Mater. 2013, 1 (1, 11002).

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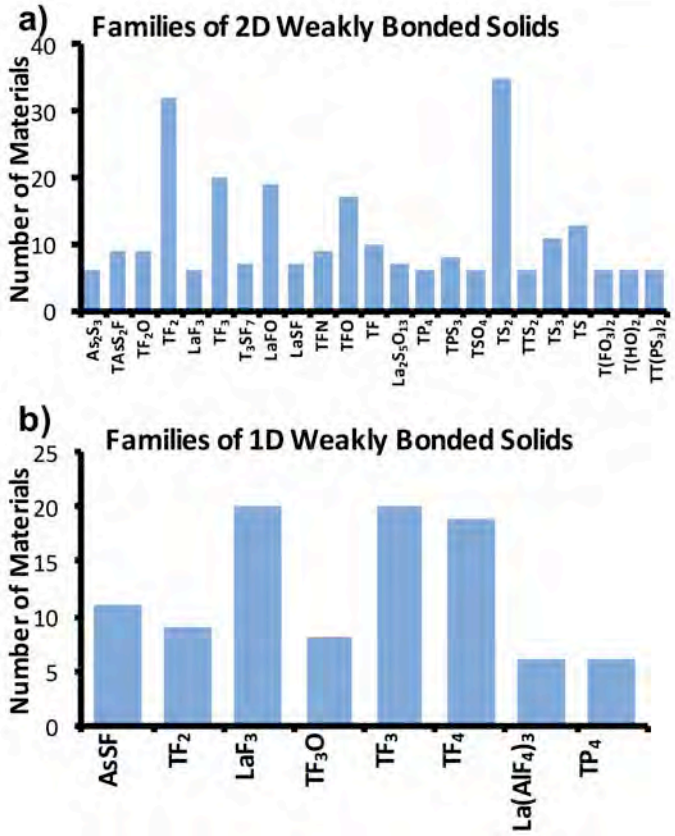

Figure 1. Histogram of families of weakly bonded solids with 2D (figure a) and 1D (figure b) subunits with similar chemical composition found in this work. Elements of the same group are represented by one symbol, with the exception of N, P, Al and O, which form families that other members of the same group do not. Ac: actinides, As: large pnictogens (As, Sb, Bi), F: halogens, S: chalcogens excluding O, La: lanthanides, T: transition metals. Only the families containing more than five materials are shown in the plot.

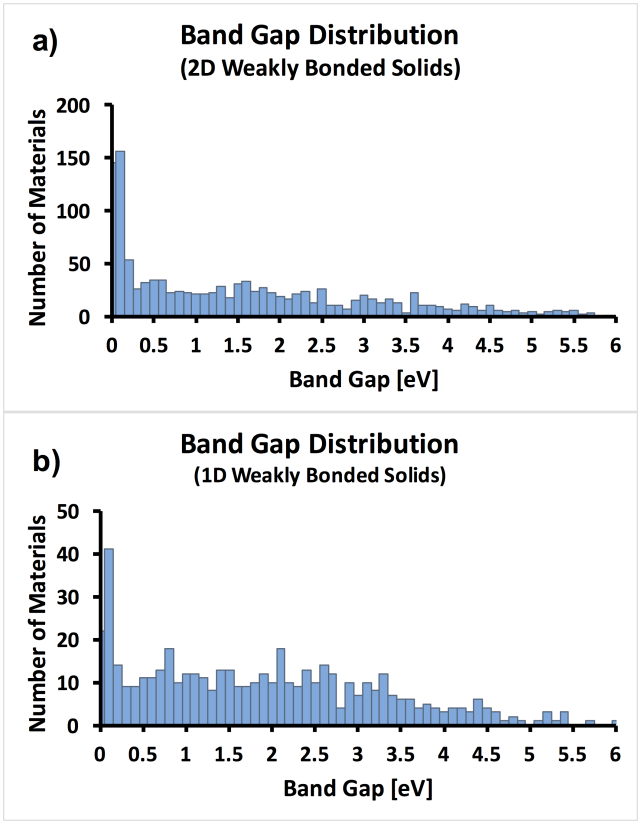

Figure 2. Distribution of semi-local DFT Kohn-Sham band gaps for bulk materials consisting of 2D layers (figure a) and 1D chains (figure b) in the Materials Project database. Shown are band gaps reported in the Materials Project database computed for the bulk crystal rather than the isolated 2D and 1D components.

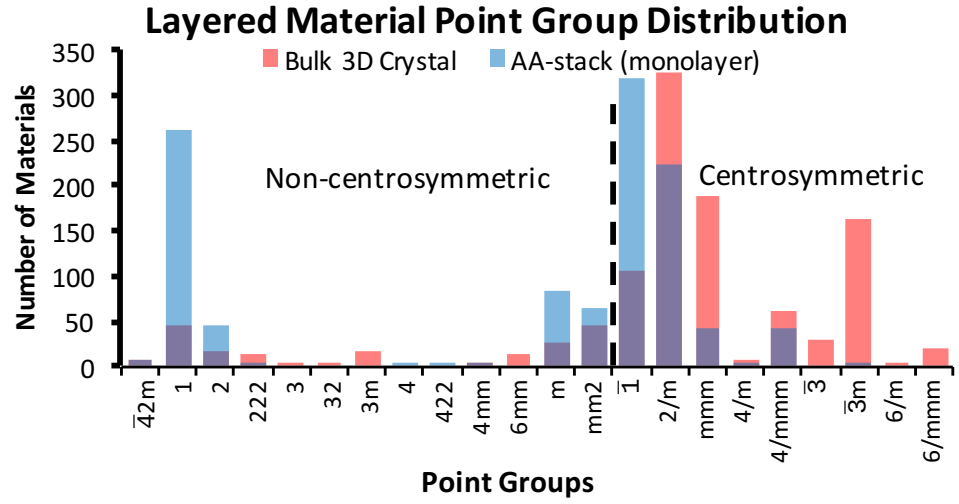

Figure 3. The point group distribution of layered materials in the Materials Project database, omitting heterostructures. If there are multiple layered phases for one material, the point group of the most energetically favorable layered structure was chosen.