Real gapped metals: when energy lowering symmetry breaking does not open the gap

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Electronic structure is one of the basic properties of solids which for a long time has been classified by the temperature dependence of the resistivity. Thus, for a metal, a temperature increase leads to enhanced atomic vibrations resulting in stronger scattering of free carriers, in experiments, such behavior results in increased resistivity with temperature. In contrast, for an insulator, an increase in temperature leads to the thermal activation of free carriers resulting in the reduction of resistivity. With the development of electronic structure theory, a unique class of materials - gapped metals - that combine the nature of both compounds has been discovered. Thus, similar to insulators, gapped metals have an internal band gap between principal band edges, while similarly for metals, they have free carriers to transport electrons. These unique compounds have recently attracted significant attention for their potential application in different areas of materials science. For instance, SrVO3 and CaVO3 are examples of "correlated" transparent conductors [1], Sr1-xNbO3 is a color photocatalyst [2], Ca6Al7O14 being the example of the first solid-state electride [3], etc. Such unique materials cannot be simply detected by the trial-and-error Edisonian approach and are usually found incidentally. Until now, such compounds have been noted within usually a broader scope of works, such as the search of different types of intermediate band compounds [4], identification of potential solid-state electrides [5], or topological semimetals [6-8]. While all these seminal works provided fundamental development to the field, they did not yet fully provide the richness of the family of gapped metals and details for their design principles. Motivated by this, in this work, using open-access databases and our high-accuracy first-principles calculations, we perform fundamental screening of the potential gapped metals. We note that many gapped metals listed in open-access databases are false metals – compounds that open the gap due to spontaneous symmetry breaking. However, some compounds are indeed stable with respect to the development of different local motifs.

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