MORE-MXenes: Magnetically Ordered Rare Earth 2D MXenes

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Abstract

Discovered in 2011, MXenes are by far the youngest family of 2D materials known and thus the least understood. MXenes are so called because they are derived from the Mn+1AXn (or MAX) phases where M is an early transition metal, A is an A-group elements, X is C and/or N. To convert the MAX phases to their MXenes, the A-layers (vast majority of which are Al) are selectively etched using HF-containing solutions. The A-layers are replaced by surface terminations, T, (-O, -OH and –F) which is why their proper designation is Mn+1XnTx.While most of the MAX phases were known in 1970, in 2014 out of plane ordered MAX phases were discovered. In 2017, one of the PI's of this proposal predicted and then synthesized quaternary compounds with the formula (M'2/3,M"1/3)2AlC, where M' and M'' are two metals, one of which is an early transition metal. What distinguishes these phases from all others is the in-plane ordering of the M' and M" atoms, which is why we are labelling them i-MAX phases. In work that is yet to be published, the same group predicted the existence of i-MAX phases with the chemical formula: (M2/3RE1/3)2AlC, where RE = Ce, Pr, Nd, Sm, Gd, Tb, Dy, Er, Ho, Tm and Lu. These phases were also predicted to be and indeed found to be magnetic with transition temperature < 10 K.Since all these phases are Al-containing, the Al should be readily selectively etched to create 2D RE-i-MXenes, where the RE elements are ordered in the basal planes. The goal of the proposed work is to fundamentally understand the electronic and magnetic properties of single RE-i-MXenes layers. The latter will be produced in two ways: i) mechanical exfoliation of large single crystals and, ii) chemical exfoliation/etching of powders. The ultimate objective is to deposit single layers on SiO2/Si substrates and characterize them. The differences in properties between the two configurations will elucidate the crucial role that surface terminations and etching induced defects play on the transport, and more importantly, magnetic properties.The work involves 4 labs: i) LMGP in Grenoble, is the only lab in the world that routinely produces large MAX single crystals. It will grow RE-i-MAX crystals and mechanically exfoliate them. ii) The Neel Institute, also in Grenoble, will concentrate on processing devices and measuring the low temperature magnetic properties of both i-MAX and RE-i-MXenes phases. iii) The Linkoping University group in Sweden will be responsible for supplying high purity powders to the other partners and continuing in their trail blazing efforts to understand the magnetism of these phases by DFT calculations. iv) The UCL group in Louvain, Belgium will measure and simulate (through ab initio calculations) transport and vibrational (Raman) properties of both the i-MAX and RE-i-MXenes materials, with a particular focus on the role of surface termination in the case of MXenes.The possibility to significantly increase the palette of available metallic MXene 2D crystals is important in the perspective of "full 2D" electronic and spintronic devices, as they could be used both as interconnects with low electrical resistivities and low contact resistances, and/or for spin injection/detection.

Consortium

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