Magnetic Nitrides as Quantum Materials

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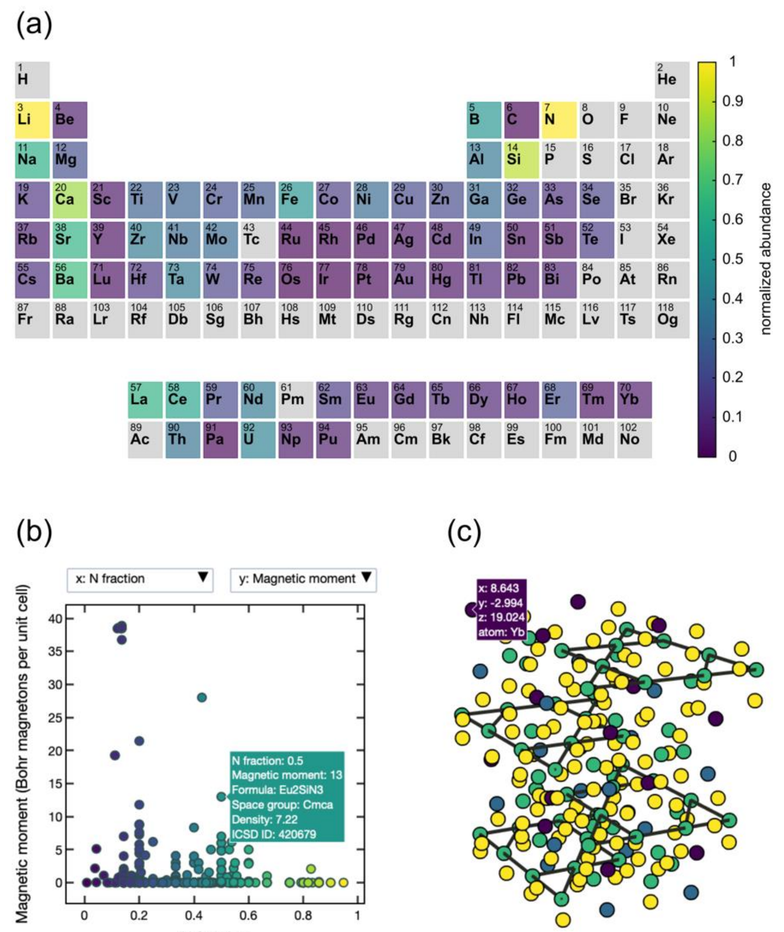
The materials class of nitrides is underexplored in comparison to oxide materials. The Inorganic Crystal Structure Database (ICSD) contains over 210000 crystal structures. Approximately 98000 (47 %) entries are structures including oxygen and only 16000 (8 %) entries contain nitrogen. Even less structures can be considered to be nitride materials (about 1100) – materials that contain nitrogen in a formal oxidation state of −3. Oxides are ubiquitous in nature as minerals. Magnetite (Fe_3O_4) and quartz (SiO_2) are oxide minerals commonly found on earth.[1] In contrast, nitride materials are rarely found in nature. For example, the nitride of silicon, Nierite (Si_3N_4), occurs naturally only in residues of primitive meteorites.[2] Especially magnetic nitrides are rarely studied.



(a) Periodic table of elements colored according to the number of times each element is found in the nitrides reported in ICSD. (b) Magnetic moment of nitrides versus the nitrogen fraction. (c) Interactive plot generated from Python code that searches crystal structures for Kagome lattices.

The nitride anion enables strong hybridization with *d* states of transition metals that can lead to strong magnetic exchange coupling. We propose to combine this effect with frustrated lattice geometries, such as triangle or honeycomb motifs, to realize magnetically frustrated quantum nitrides. Here, we report on the data-driven analysis of reported nitride crystals structures and the selection of quantum nitride candidate materials. Furthermore, we report on progress in crystal growth attempts of a series of skyrmion host nitrides in the filled β-Mn structure, $FePd_{1-x}Pt_xMo_3N$.[3] We are employing high nitrogen gas pressures in a unique laser floating zone furnace to stabilize nitride compounds in the molten state to enable nitride single crystal growth.

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References:

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