Datamining of Magnetic Double Perovskites

MICHELE VISCARELLI[1,2], THOR WIKFELDT[1,3,2], ANNA DELIN[1,2,3]

[1] Department of Applied Physics, School of Engineering Sciences, KTH Royal Institute of Technology, Electrum 229, SE-16440 Kista, Sweden
[2] SeRC (Swedish e-Science Research Center), KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden
[3] PDC Center for High-Performance Computing, KTH, Stockholm
[4] Department of Physics and Astronomy, Materials Theory Division, Uppsala University, Box 516, SE-75120 Uppsala, Sweden

Scope:
Double perovskites (DPs) are a very versatile class of materials with chemical formula A,B'B''O₆. A clever choice of B',B'' opens up the possibility of new interesting materials [1,2]. The number of possible combinations of A, B', B'' is enormous, and many of them have never been studied or synthesized [2]. Inside this “uncharted territory” there are double perovskites that can show interesting features. We employ a data-driven, high-throughput computational framework for the study of a subset of double perovskites, with A = Sr, with B' among 3d, 4d and 5d elements, with the goal to predict their chemical stability.

Formation energies calculations:
● AiiDA open-source materials’ informatics infrastructure [3] for calculations submission, data storage and data analysis
● DFT structural and ground state calculations with QuantumESPRESSO
● Pure elements structures from Materials Project DB [4]
● Cubic double perovskites' structures.
● Automated calculation of formation energies

Stability prediction:
● Focus on Ir-based double perovskites
● Materials Project database querying for competing stable phase structures
● Formation energy calculations for all the retrieved competing phases at the same level of theory as double perovskites calculations (~ 3000 calculations)
● Construction of the convex hull of stability given all the information
● Data compared with [2] when available

Results:
● Formation energies (d) increases moving along the Periodic Table due to A, B', B'' cation size
● Distances from hull (c) lay very close to the stability limit of 0.0 meV/atom.
● 6 new predicted stable Ir-based double perovskites, plus 2 quasi-stable (distance from hull < 30 meV/atom)
● B' = Mn, Fe, Co, Ni are the ones with the least robust stability, with distances from hull less than 50 meV/atom.
● Cubic structure to describe Ir-double perovskites is a good approximation for stability predictions.
● B' = Al, Ti, V, Zr, Hf, Ta with non magnetic ground state.

References