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HOW MANY MATERIALS ARE LEFT TO DISCOVER? AN EXPLORATION OF QUATERNARY SPACE

M. Sluydts[1,2], M. Larmuseau[1,2], T. Crepain[1], K. Dumon[1], K. Lejaeghere[1,3] and S. Cottenier[1,2]

[1] Center for Molecular Modeling, Ghent University, Belgium
[2] Department of Electrical Energy, Metals, Mechanical Constructions & Systems, Ghent University, Belgium
[3] Department of Applied Physics, Ghent University, Belgium
email: michael.sluydts@ugent.be

The frontier of materials science is shifting evermore towards the development of 'exotic' functional materials, which display an unfamiliar combination of properties. The underlying behavior giving rise to these materials' properties is often too complex to predict purely from their crystal structure. New exotic materials are thus largely developed by mimicking existing materials, inevitably introducing bias.

While truly new exotic materials are likely to exist in unknown regions of materials space, it is unlikely we will find them through biased exploration. At the same time, random exploration is unsustainable given the time required to synthesize and characterize new materials. Several questions thus arise. How can we explore the vast materials space intelligently, yet without bias? And perhaps most importantly: how many materials are left to discover?

We investigate this fundamental question by creating a database of hypothetical crystals in quaternary space, where experimental exploration is limited. By employing high-throughput ab initio methods, we are able to predict various properties of these unknown materials, including their stability. Furthermore, applying machine learning during the screening procedure yields a ten-fold speedup over brute-force exploration. This yields a relatively unbiased, yet fast exploration method.

By comparing the discovery rate, composition and structure of the new materials with that of experimentally known quaternary phases, an estimation can be made of how many materials are yet to be discovered within this region of materials space.