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Mapping the ICSD

Tuesday 9 April 2024 18:30 (20 minutes)

In this talk, I will discuss mapping the inorganic materials that have been reported in the ICSD [1]. This is important for both Materials Genome Initiative (MGI) [2] approaches to finding new materials and for adequately judging the uncertainty in machine learning approaches to structural determination from diffraction data.
We use a measure of structure similarity to determine how similar one crystal structure is to another. Given this similarity measure, we use community detection methods [3] and hierarchal clustering to find families of structurally similar materials. We demonstrate results from a small sampling of the ICSD. In the future, we will expand this to cover the entire database.

[1] NIST Inorganic Crystal Structure Database, NIST Standard Reference Database Number 3, National Institute of Standards and Technology, Gaithersburg MD, 20899, DOI: https://doi.org/10.18434/M32147

[2] National Science and Technology Council, Materials Genome Initiative Strategic Plan (Nation-al Science and Technology Council, 2014), https://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/mgi_strategic_plan_-_dec_2014.pdf.

[3] Community Detection in Graphs, Santo Fortunato, Physics Reports 486, 75 (2010). https://doi.org/10.1016/j.physrep.2009.11.002

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