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Automatic high-throughput screening of colloidal crystals using machine learning MATTHEW SPELLINGS, SHARON C. GLOTZER, Univ of Michigan - Ann Arbor — Recent improvements in hardware and software have united to pose an interesting problem for computational scientists studying self-assembly of particles into crystal structures: while studies covering large swathes of parameter space can be dispatched at once using modern supercomputers and parallel architectures, identifying the different regions of a phase diagram is often a serial task completed by hand. While analytic methods exist to distinguish some simple structures, they can be difficult to apply, and automatic identification of more complex structures is still lacking. In this talk we describe one method to create numerical "fingerprints" of local order and use them to analyze a study of complex ordered structures. We can use these methods as first steps toward automatic exploration of parameter space and, more broadly, the strategic design of new materials.

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