



# CMCC *Mechanochemistry Discussions*

Online Seminar Series

## Stochastic Sampling of Material Structure Space

Livestreaming at  
10:00 AM (CT)

THURS., April 15, 2021

on the CMCC YouTube Channel:  
[Dr. Chris Pickard Seminar](#)



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### ABSTRACT:

Over the last decade, high pressure and materials research has been transformed by the ability to predict both the structures and properties of materials from first principles. In many cases these predictions have been later confirmed by experiment. In others they have provided fruitful new directions to explore.

This progress has been achieved through the combination of stochastic approaches with reliable and efficient first principles methods. Diverse ensembles of initial structures can be generated, and structurally optimized. The resulting low energy structures are candidates for stable, and metastable, phases and/or defects and interfaces that might be experimentally realized. Success, of course, depends on a sufficiently broad and thorough sampling of configuration space.

A purely random strategy, as employed by Ab Initio Random Structure Searching (AIRSS), [1,2] is entirely parallel, and a natural fit to the high throughput computation (HTC) paradigm. Challenging cases can be tackled by designing the initial random structures so that they focus the search in regions of configuration space that are anticipated to yield success.

The design of these random “sensible” structures will be explored, along with some new directions [3] which promise to help our understanding of, and accelerate random search, along with applications to high pressure and materials research – from dense hydrides approaching room temperature superconductivity, to surprising astrophysical reactions and complex interfacial materials.

References:

[1] C. J. Pickard, and R. J. Needs, Phys. Rev. Lett., 97 (4), 045504 (2006) & JPCM, 23(5), 053201 (2011)

[2] Released under the GPL2 license: <http://www.mtg.msm.cam.ac.uk/Codes/AIRSS>

[3] C. J. Pickard, “Hyperspatial optimization of structures”, Phys. Rev. B, 99, 054102 (2019)



The CMCC is supported by the Division of Chemistry of the National Science Foundation under grant: 2023644.



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