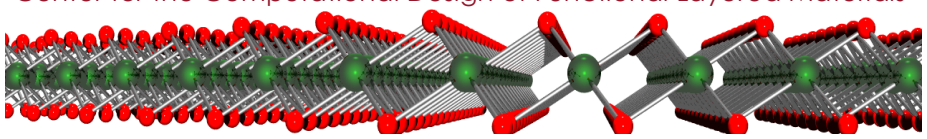
Center for the Computational Design of Functional Layered Materials



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Synthesis, the new frontier for computational materials science

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The ab-initio prediction of properties has made tremendous progress in the last three decades, making it now possible to predict many functional properties of compounds with high reliability. This has led to many examples of computer-designed materials.

As computational property prediction continues to extend its reach, we will become increasingly limited by the time required needed to synthesize new materials in a predictive and controlled manner. In particular, an understanding of which metastable compounds can be formed and under which condition they can be made would enhance the focus on computational materials design towards feasible, synthesizable materials.

I will discuss the scientific ideas that can lead to a predictive theory of synthesis, and give several examples where the synthesis path for metastable compounds can be predicted. In addition, I will also highlight recent ideas in using artificial intelligence methods and machine learning to learn materials synthesis.

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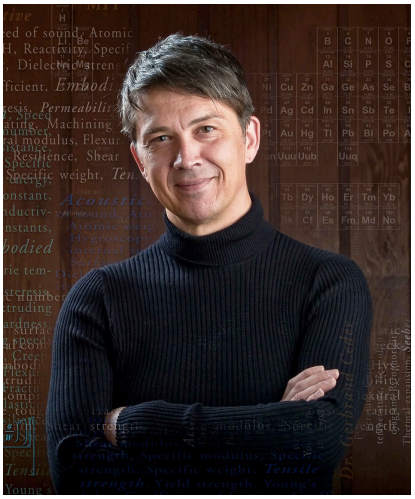

Gerbrand Ceder is The Chancellor's Professor of Materials Science and Engineering at UC Berkeley. His research interests lie in computational and experimental materials design for clean energy technology and in Materials Genome approaches to materials design and synthesis. He has published over 400 scientific papers, and holds more than 20 U.S. and foreign patents. He is a member of the National Academy of Engineering of the US and the Royal Flemish Academy of Belgium for Science and The Art. He is a Fellow of the Materials Research Society and the Metals, Minerals and Materials Society, and has received awards from the Electrochemical Society, the Materials Research Society, the Metals Minerals and Materials Society, and the International Battery Association. He is a Lead Scientist for new battery technologies at the Joint Center for Energy Storage (JCESR) of the US Department of Energy, and the Chief Scientist of the Energy Frontier Research Center at the National Renewable Energy Laboratory