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Meta-Stable Materials Lab

Decoding Materials for a Sustainable Future …

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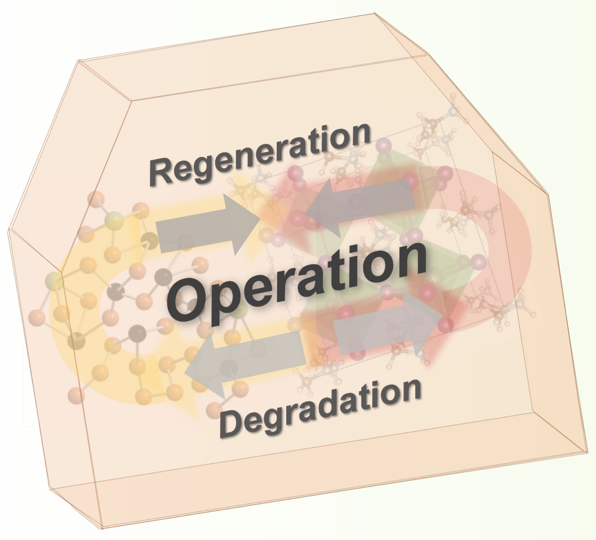
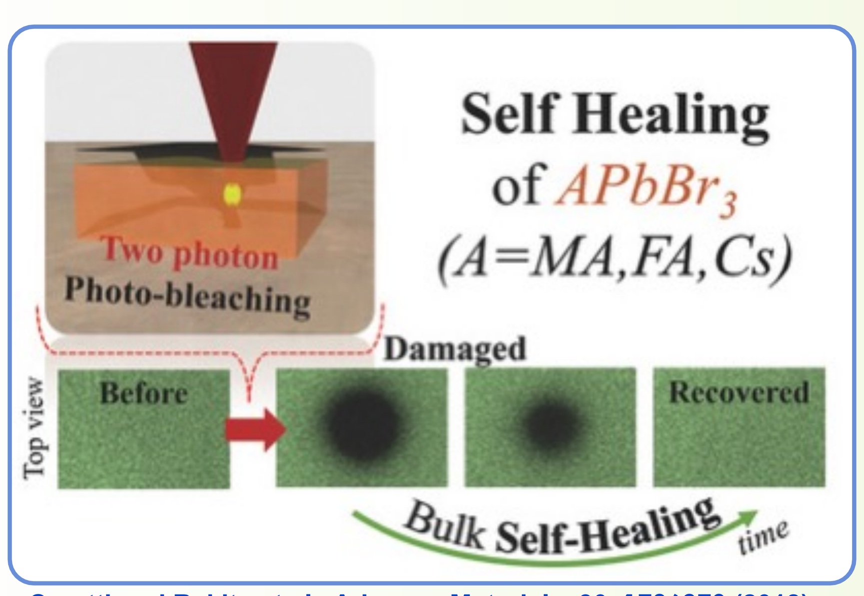
Meta-stable and Regenerative materials



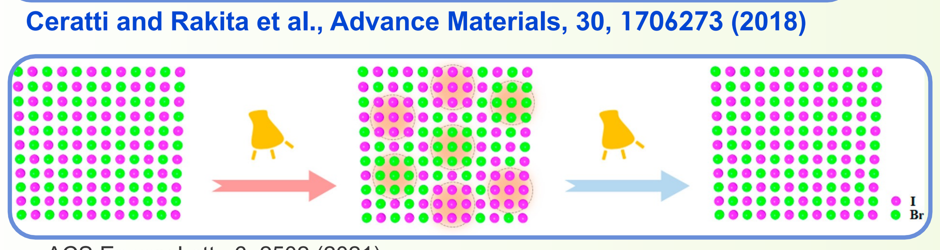
Meta-stable materials provide an extension to the properties and functionalities of (thermodynamically) stable materials. They are dynamically formed during transition between states, where if the dynamics of the formation process is reversible, they can be also called **Regenerative** materials.

In our lab we focus on regenerative materials and on the understanding and stabilization of their different meta-stable states. We target halide perovskites (HaPs) and phase-change materials (PCM) as *regenerative* functional materials. Our main objective is to understand their transformation between meta-stable states, and the stabilization of desired meta-stable states.
We develop these understandings for neuromorphic computation applications, and energy recycling, harvesting and storage applications. Our task is to decode their properties and structural complexity towards their understanding and rational design.

Halide Perovskites (HaP) compounds (ABX_3, X=halide) show, on the one hand, structural instability during normal operation conditions (illumination, applied bias), but also spontaneous self-healing. We study the degradation and regeneration dynamics and ways to control it.

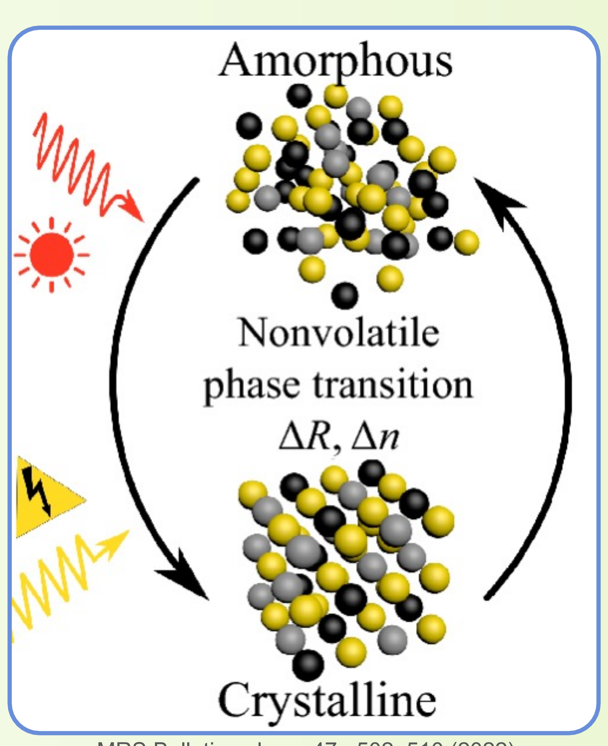


Ceratti and Rakita et al., Advance Materials, 30, 1706273 (2018)



ACS Energy Lett., 6, 2502 (2021)

Phase Change Materials (PCM), e.g. $Ge_2Sb_2Te_5$, strongly change their optical and electrical properties upon switching between an amorphous to crystalline phase. Being an unusually fast phase-transformation, the switching process lacks understanding.

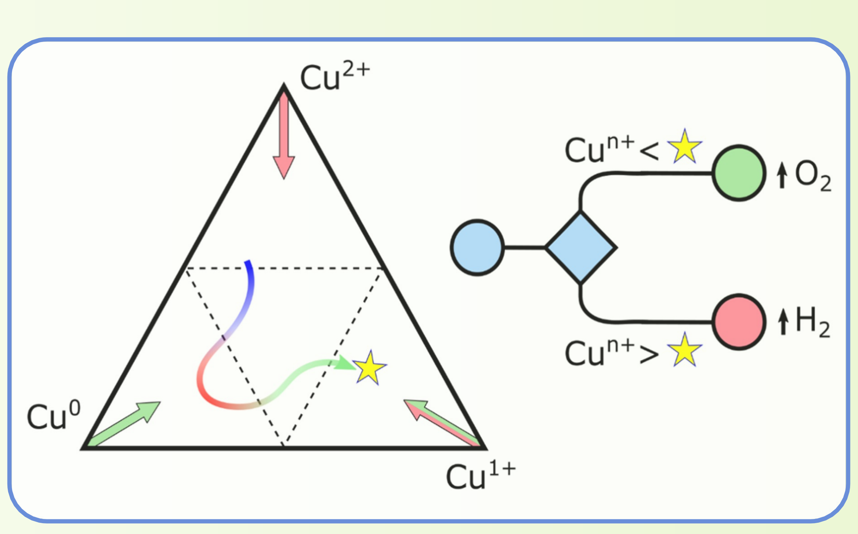


MRS Bulletin volume 47, 502–510 (2022)

Active reaction control of meta-stable materials

We develop an **autonomous** navigation infrastrucutre for complex chemical systems, where we use machine-learning to reach a targeted meta-stable state during solid-state synthesis.

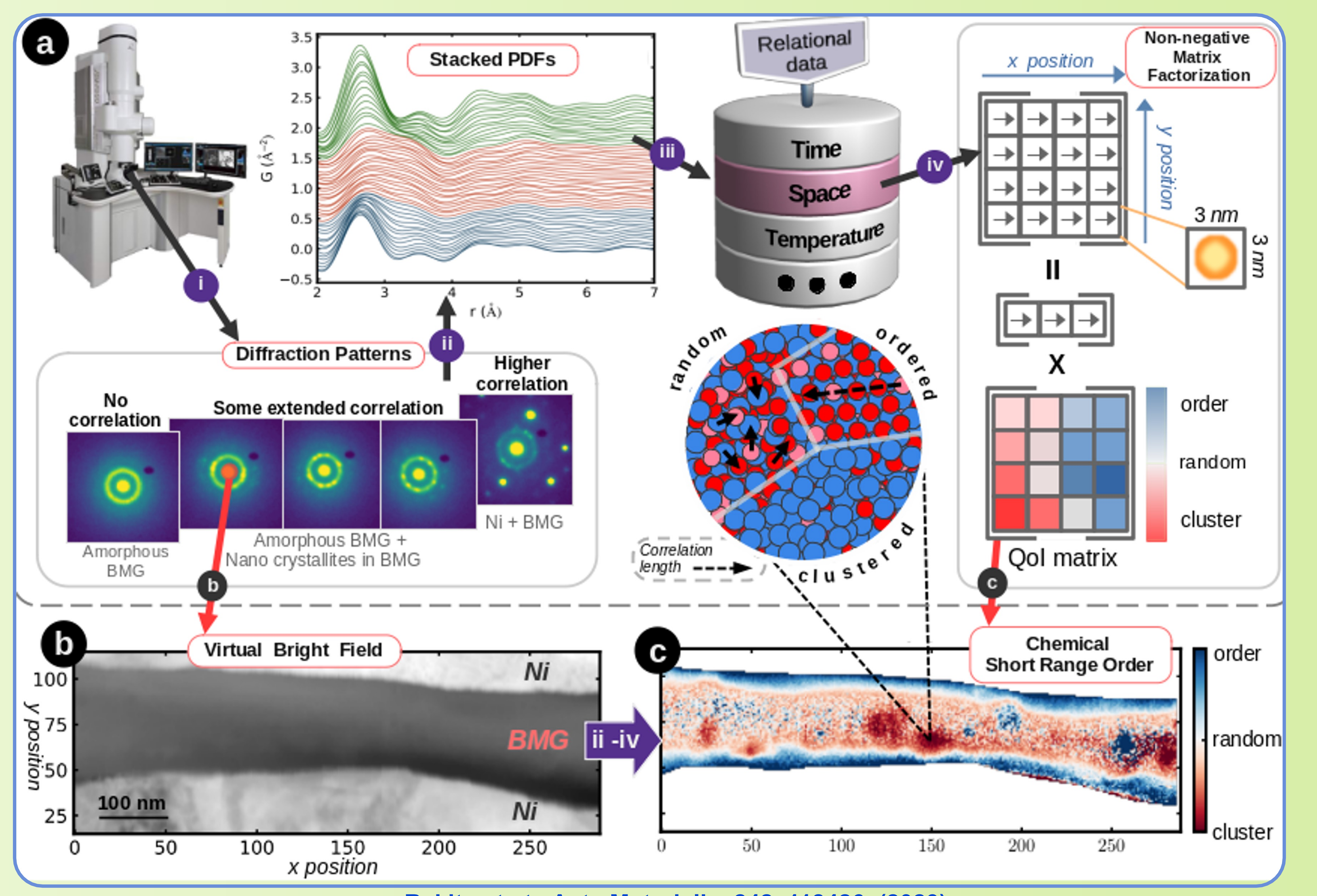
To navigate in a complex chemical space, such as during the formation of meta-stable materials, we develop a self-navigated (autonomous). infrastructure to control formation of meta-stable states. The infrastructure actively controls the synthesis parameters and timing based on measured quantity of-interest (QoI). We target fragile glass-forming materials and phase change materials (PCM). We harness event-model principles and Machine Learning (ML) tools, such as 'reinforcement learning', to provide a self-evolving recommendation system for synthesis parameters.



Rakita and O'Nolan JACS, 142, 18758 (2020)

Machine-Learning-assited evolution mapping of meta-stable structres

We develop nano-meter resolution machine-learning (ML) based analysis for disentangling structural order in meta-stable structures.
Combining ML-tools with relational diffraction data from scanning transmission electron microscope (4D-STEM), we develop the Scanning Nano-Structure Electron Microscope (SNEM) technique. - a tool for mapping the local ordering distribution and its evolution at the nano-scale resolution. The development of SNEM should provide an insight to nano-meter-sized structural events in meta-stable systems, which previously believed to be uniform due to lack in probing resolution and efficient data analysis, which are available today.

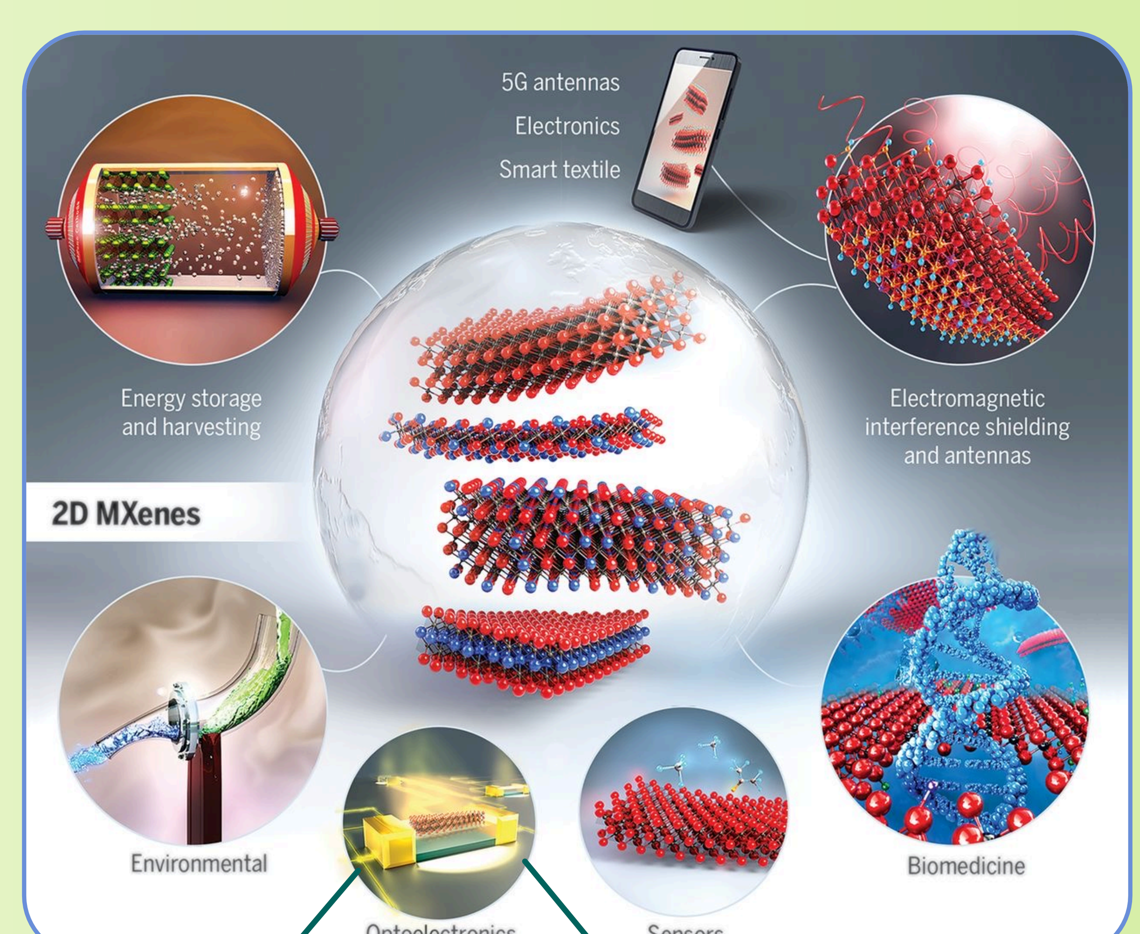


Rakita et al., Acta Materialia, 242, 118426 (2023)

Tuning meta-stable materials using MXenes

MXenes are **2D** transition metal (***M***) carbides/nitrides (***X***) with a termination group (**T**) (e.g. $Ti_3C_2T_x$ or Ti_2CT_x).

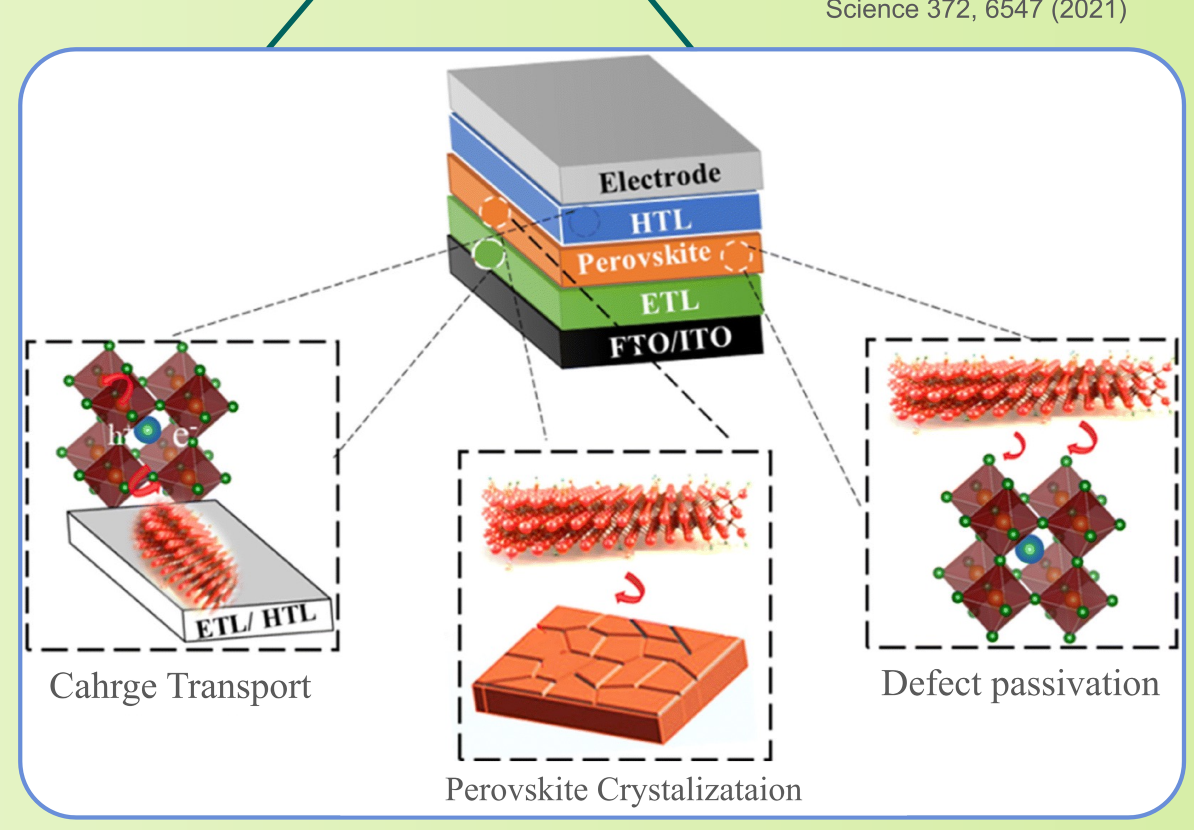
They show many intriguing properties, including chemical flexibility and high surface area, which make them both tunable by their chemical environment and capable of affecting the stability of surrounding meta-stable systems.



Science 372, 6547 (2021)

Our **goals** are to:

- Understanding the chemical activity of MXenes with *poly*-halides as a platform to control meta-stable systems.
- Understanding interactions between MXenes and Halide-Perovskites to rationalize solar element design for better performance, stability and reproducibility.



Nanoscale, 14, 13018 (2022)