How to discover new solids containing alkali metals: predictive screening, facile synthesis and in situ studies

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Materials discovery can be accelerated by the development of synthesis methods and in-situ characterization techniques allowing for the rapid "screening" of multicomponent systems, while theoretical predictions of new compounds' structure and thermodynamic stability can yield the desired roadmap for the targeted synthesis. However, the sluggish kinetics of solid-state reactions entails the necessity of high temperatures and long annealing times, often leading to the stabilization of the thermodynamically stable products. We are interested in unconventional synthesis methods toward solid-state materials, using reactive, salt-like precursors. Our synthesis is guided by real-time reaction monitoring and theoretical predictions. I will show how new ternary compounds containing alkali metals (Li, Na, K) can be discovered using this approach. I will further discuss their structural features established by comprehensive diffraction methods, and physical properties.