AI and autonomous laboratories for materials synthesis

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Computational materials science has seen tremendous progress since the early days of Density Functional Theories. Stable algorithms enabled high-throughput computing which in turn enabled machine-learned potentials (MLP). Though far from perfect at this point, MLPs hold tremendous promise for accelerating materials simulation and discovery.
Such progress is not parallelled on the experimental side, making it the gating factor in materials development. In response we built, A-lab, an autonomous facility for the closed-loop synthesis of inorganic materials from powder precursors. All synthesis and characterization actions in A-lab, including powder mixing and grinding, firing, characterization by XRD and SEM, and all sample transfers between them are fully automated, leading to a lab that can synthesize and structurally characterize compounds within 10-20 hrs of initiation. The A-lab leverages ab-initio computations through an API with the Materials Project, historical data sets that are text-mined from the literature, machine learning for optimization of synthesis routes and interpretation of characterization data, and active learning to plan and interpret the outcomes of experiments performed using robotics. The automation of synthesis and analysis can be further integrated into scientific workflows similar to computational workflows