

Combining machine learning and automation to accelerate sustainable materials development

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Abstract:

Machine learning (ML) has emerged as an essential tool for rapidly designing new materials with desired properties. In this context, an ML model may be employed within an iterative sequential learning (SL) loop to prioritize candidate materials, so that only the most promising candidates are investigated further via experiments or physics-based simulations. The results of these experiments or simulations are then used to re-train the ML model, and the SL loop repeats.

Such an SL workflow is very efficient at identifying high-performing materials. However, SL is sensitive to the cycle time per iteration, or the delay between ML predictions and experimental or computational feedback. This state of affairs has driven intense interest in the use of automation to significantly accelerate the overall SL process. In this talk, I will discuss some sustainability-related examples of combining automation (both experiments and simulations) with SL.