Accelerating materials discovery through machine learning

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Advanced materials are critical for modern technologies and a sustainable future. However, discovery, design, and synthesis of novel advanced materials (especially those containing three or more elements) with desired functionalities is of great challenge because the number of possible combinations in the composition-structure-property space is enormous and complex. We have developed a machine learning (ML) guided framework by efficiently integrating deep ML with the state-of-the-art computational methods, database, and experimental validations to tackle this grand challenge problem. Our ML-guided framework greatly reduces the complicity of the problem and makes *ab initio* calculations and structure search algorithms much more effective, thus dramatically accelerating the pace of materials discovery. Studies on the discovery of high performance rare-earth free magnetic materials and novel complex quantum materials will be presented. The challenges in closing the feedback loop between computational prediction and experimental synthesis will also be discussed.

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