Towards an Efficient Exploration of the Materials Design Space

Over the last decade, there has been a paradigm shift away from labor-intensive and time-consuming materials discovery methods, and materials exploration through informatics approaches is gaining traction at present. Current approaches are typically centered around the idea of achieving this exploration through high-throughput (HT) experimentation/computation. Such approaches, however, do not account for the practicalities of resource constraints, which eventually result in bottlenecks at various stages of the materials discovery/design workflow. Regardless of how many bottlenecks are eliminated, the fact that ultimately a human must make decisions about what to do with the acquired information implies that HT frameworks face hard limits that will be extremely difficult to overcome. Recently, this problem has been addressed by framing the materials discovery process as an optimal experiment design problem. In this talk, I will discuss the need for optimal experiment design, the challenges in its implementation and finally discuss some successful examples of materials discovery via experiment design. Specifically, I will discuss some recent examples in which my group and collaborators have demonstrated: (i) Multi-objective materials discovery and design; (ii) Bayesian optimization under model uncertainty (BOMU); (iii) Multi-source information fusion Bayesian optimization for materials design; (iv) Batch Bayesian optimization applied to microstructure sensitive design of materials.

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