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**High-Throughput Computational Design of Advanced Functional Materials: Topological Insulators and Two-Dimensional Electron Gas Systems**  
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As a rapidly growing area of materials science, high-throughput (HT) computational materials design is playing a crucial role in accelerating the discovery and development of novel functional materials. In this presentation, I will first introduce the strategy of HT computational materials design, and take the HT discovery of topological insulators (TIs) as a practical example to show the usage of such an approach. Topological insulators are one of the most studied classes of novel materials because of their great potential for applications ranging from spintronics to quantum computers. Here I will show that, by defining a reliable and accessible descriptor, which represents the topological robustness or feasibility of the candidate, and by searching the quantum materials repository [aflowlib.org](http://aflowlib.org), we have automatically discovered 28 TIs (some of them already known) in five different symmetry families. Next, I will talk about our recent research work on the HT computational design of the perovskite-based two-dimensional electron gas (2DEG) systems. The 2DEG formed on the perovskite oxide heterostructure (HS) has potential applications in next-generation nanoelectronic devices. In order to achieve practical implementation of the 2DEG in the device design, desired physical properties such as high charge carrier density and mobility are necessary. Here I show that, using the same strategy with the HT discovery of TIs, by introducing a series of combinatorial descriptors, we have successfully identified a series of candidate 2DEG systems based on the perovskite oxides. This work provides another exemplar of applying HT computational design approach for the discovery of advanced functional materials.