Data-driven discovery of novel materials for smart optoelectronics

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1. AI in materials science

In recent years, the demand for novel materials and for methods enabling the design of materials with targeted properties has grown rapidly. Increasing industrial requirements for performance and quality, combined with the high cost and limited throughput of experimental discovery, have driven the development of computational materials science and materials informatics. Traditionally, new materials were identified primarily through experimental trial-and-error, guided by expert intuition and prior results, a process that is time-consuming, resource-intensive, and dependent on specialized facilities and human expertise. Over the past approaches have matured, enabling accurate prediction of material structures and properties prior to synthesis or testing. The integration of artificial intelligence has further accelerated this paradigm shift: large-scale materials databases, machine-learning models for property prediction, and generative algorithms for designing novel compounds now enable a systematic, data-driven approach to materials discovery, substantially improving both its efficiency and scope.

In this talk, we demonstrate how these AI-driven methodologies are transforming the design of smart electronic devices, with a particular focus on data-driven discovery of functional materials for next-generation smart contact lenses.

2. How AI changes the way of materials discovery

The exploration of van der Waals (vdW) materials, renowned for their unique optical properties, is pivotal for advanced photonics. These materials exhibit exceptional optical anisotropy, both in-plane and out-of-plane, making them an ideal platform for novel photonic applications. However, the manual search for vdW materials with giant optical anisotropy is a labor-intensive process unsuitable for the fast screening of materials with unique properties. Here, we collected a database of vdW materials and their optical properties [1-3] and trained graph neural network to predict their birefringence with close to ab initio accuracy. Experimental verification with 2H-MoTe2 and CdPS3 confirms the theoretical predictions, underscoring the potential of ML in discovering and optimizing vdW materials with unprecedented optical performance [4].

To bridge the gap between theory and experiment, we further developed a physics-guided ML framework that integrates DFT, graph neural networks, experimental methods, and Cauchy-model corrections. Using a database of over 1000 two-dimensional materials, we enable reliable prediction of refractive indices in the near-infrared range while introducing a physically meaningful definition of 2D thickness. The resulting models capture structure–property relationships with high fidelity and enable rapid screening of monolayers with tailored optical functionalities [5]. This approach is exemplified by identifying high-index candidates such as Bi_2Te_2Se, which enable enhanced field confinement in integrated photonic devices (Figure 1).

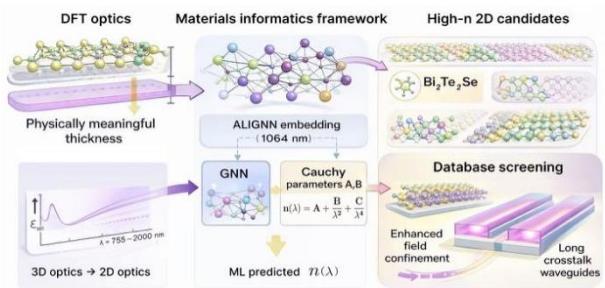

Fig. 1: Physically informed ML model for the search of novel 2D materials with target optical properties

We also introduce an AI-driven framework for predicting substrate-stabilized 2D structures by integrating evolutionary optimization, lattice matching, automated training of machine-learning interatomic potentials, and *ab initio* thermodynamics. Applied to the Mo–S system on c-cut sapphire, this approach uncovers multiple stable and metastable phases, including

1H-MoS_2 and previously unknown compounds such as Mo_3S_2, Mo_2S, Mo_5S_3, and Mo_4S. These results establish a route toward computational substrate engineering, enabling predictive control over the stability and functional properties of 2D materials and providing practical guidance for their experimental synthesis [6].

Overall, these results demonstrate how physics-informed AI enables a transition from empirical trial-and-error to predictive, data-driven materials design across multiple scales. By unifying *ab initio* modeling, machine learning, and experimental validation, this paradigm provides a foundation for the rational discovery of functional materials that will underpin the next generation of photonic and electronic devices.

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