AI-guided search for bulk and 2D materials with target optical properties

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The optical properties of bulk and two-dimensional (2D) materials are fundamental to the development of modern photonic devices, such as atomically thin lenses and waveguides, ultrasensitive biosensors, high-Q resonators, and tunable metasurfaces, among others. Among these properties refractive index and birefringence play a key role. As a result, natural materials with giant anisotropy ($\Delta n > 1$) are in growing demand both for scientific and industrial purposes. In this regard, transition-metal dichalcogenides (TMDCs) in a bulk and 2D configurations are promising candidates because of their strongly anisotropic vdW structure, which naturally leads to a large intrinsic birefringence [1-3].

ML methods can boost the search for materials with high refractive index and optical anisotropy. In this work, we trained ALIGNN graph neural network to predict these properties based only on crystal structure and composition (Figure 1) [4-5]. To train ML models, we collected unique databases of known layered van der Waals and 2D materials, which consisted of their crystal structures and optical properties, calculated in density functional theory (DFT) and for some of them measured using scanning ellipsometry. In the databases, theoretically calculated and experimentally measured optical constants are in perfect agreement.

Therefore, we developed machine learning models, which can predict birefringence of bulk materials and refractive index of 2D materials with accuracy, close to DFT methods, but with a much higher speed. This allowed us to screen the existing databases of crystalline and 2D materials (MaterialsProject and C2DB) and we found novel candidate materials with target optical properties, which were then confirmed in DFT and GW calculations and experimental measurements.

References

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Figures

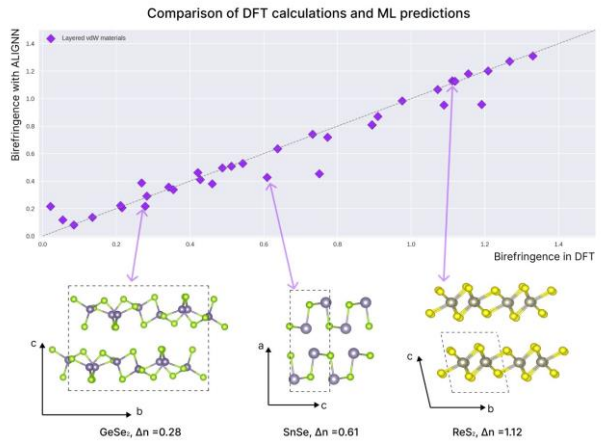

Figure 1: Machine learning model to predict birefringence of layered van der Waals materials