AI-guided screening of van der Waals materials with high optical anisotropy

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Large optical anisotropy observed in a broad spectral range is of paramount importance for efficient light manipulation in countless devices. 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 configuration are promising candidates because of their strongly anisotropic vdW structure, which naturally leads to a large intrinsic birefringence [1-4].

ML methods can boost the search for materials with high optical anisotropy. In this work, we trained ALIGNN graph neural network to predict birefringence of materials based only on their crystal structure and composition (Figure 1) [5]. Average error on test and validations sets was 0.02. To train this model, we collected a unique database of known layered van der Waals 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 database, theoretically calculated and experimentally measured optical constants are in perfect agreement.

Therefore, we developed a machine learning model, which can predict birefringence of materials with accuracy, close to DFT methods, but with a much higher speed. This allowed us to screen the existing databases of crystalline materials (MaterialsProject and GNOMe) and we found novel candidate materials with high optical anisotropy, which was then confirmed in DFT and GW calculations and experimental measurements.

References

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Figures

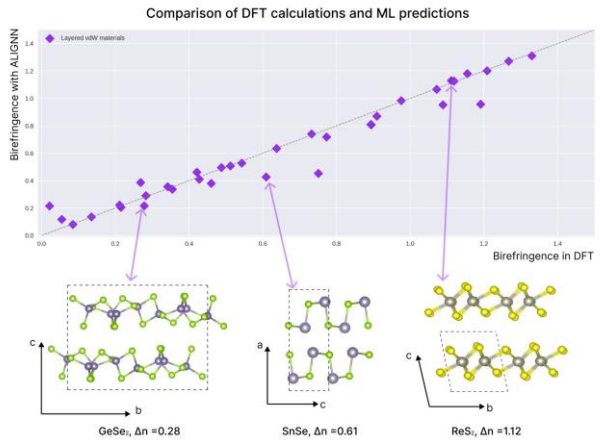

Figure 1: Machine learning model to predict birefringence of layered van der Waals materials