Data-driven discovery of van der Waals materials with high optical anisotropy

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Large optical anisotropy over a wide spectral range is crucial for effective light control in numerous photonic devices. Consequently, there is a growing need for natural materials exhibiting giant anisotropy ($\Delta n > 1$) to meet both scientific and industrial demands. In this context, bulk transition-metal dichalcogenides (TMDCs) stand out as highly promising candidates, thanks to their inherently anisotropic van der Waals (vdW) layered structures that naturally give rise to significant intrinsic birefringence [1-2].
In our study, we trained an ALIGNN graph neural network to predict the birefringence of materials solely from their crystal structures and elemental compositions (Figure 1). To achieve this, we collected a database of known layered vdW materials, including their crystal structures and optical properties calculated from density functional theory (DFT) and, for a subset of samples, from experiment. Next, we screened crystalline materials databases (MaterialsProject and GNoME) and identified new candidate materials exhibiting high optical anisotropy. Subsequent DFT calculations and experimental measurements confirmed our predictions, demonstrating the effectiveness of the developed approach in uncovering novel anisotropic materials [3].

References

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Figures

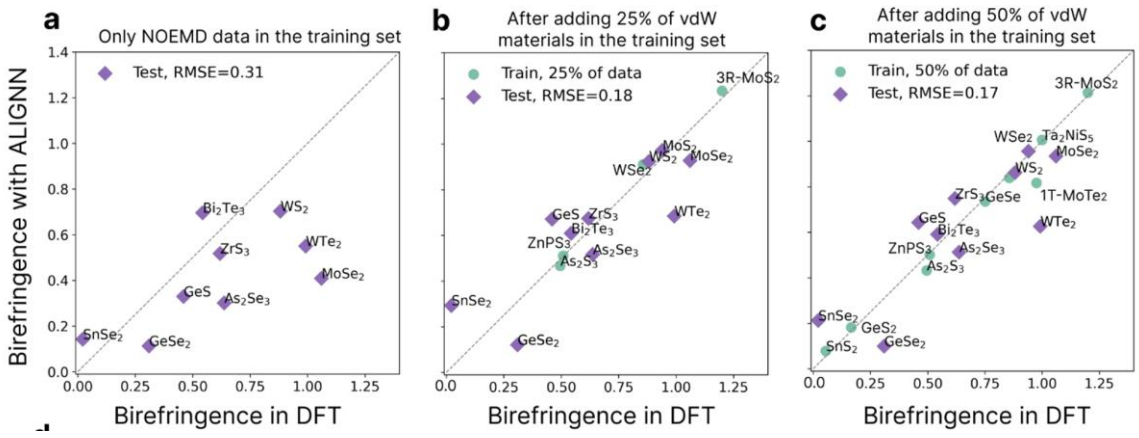

Figure 1: Comparison of ALIGNN- and DFT- calculated birefringence for vdW materials.