CrystalDFT: Sustainable Crystal Piezoelectrics Screening

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ABSTRACT

Organic molecular crystals are an emerging class of eco-friendly piezoelectric materials that are both biocompatible and biodegradable enabling their use in Lead-free biomedical applications and smart devices while ensuring eco-friendly production and disposal. The vast majority of organic materials naturally lack a centre of symmetry in their crystal structure, endowing them with piezoelectric properties. In these non-centrosymmetric crystals, a surface charge is generated under an applied force due to ionic displacement. Advances in highperformance computing have facilitated the use of quantum mechanical calculations to predict a variety of electromechanical properties including full piezoelectric tensor of molecular crystals. High-throughput density functional theory (DFT) based crystal screening employs computational methods to rapidly assess the electronic and structural properties of numerous crystal structures. Through the implementation of high-throughput screening, we have successfully conducted a comprehensive computational analysis of organic molecular crystals and their predicted electromechanical properties. This effort has resulted in the creation of a CrystalDFT database (https://actuatelab.ie/CrystalDFT) that can be used as a base for training machine learning models. We highlight the broad range of electromechanical properties amongst the simulated organic crystal dataset, and in particular, the high number of crystals that have a naturally occurring longitudinal d_{33} constant. This longitudinal electromechanical coupling is a prerequisite for several conventional sensing and energy harvesting applications, the presence of which is notably rare amongst the literature on biomolecular crystal piezoelectricity to date.

References

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