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In silico Engineering of Piezoelectric Biomolecular Assemblies

The ability of certain materials to generate electric charge in response to mechanical stress is derived from their non-centrosymmetric crystal structures, which produces a wide array of applications in sensing, actuation, and energy harvesting1. Organic molecular crystals, characterized by their structural tunability, sustainability, and biocompatibility, present a promising platform for the next generation of piezoelectric materials2. Utilizing crystal engineering and Density Functional Theory (DFT), we have developed CrystalDFT - a structured database of crystals accompanied by predicted electromechanical properties3. This dataset reveals a diverse range of piezoelectric responses, featuring a considerable number of materials exhibiting natural (unpoled) longitudinal piezoelectricity, which is essential for conventional piezoelectric applications. A focused study was also carried out on hydrated organic crystals, performing a high-throughput DFT screening and identifying thirty hydrates with longitudinal piezoelectric coefficients exceeding 10 pC/N, including one material achieving an impressive 386 pC/N. These results underscore the significance of hydrogen bonding in enhancing dipole alignment and facilitating polar crystal phases. These results led us to further investigate structure - property relationships, whereby we designed and synthesized a series of halogenated pyridin-3-ol derivatives (2-X-pyridin-3-ol; where X = Cl, Br, I). These crystals, stabilized by both hydrogen and halogen bonding4, demonstrate high DFT-predicted shear piezoelectric responses of up to 99.19 pC/N. Experimentally-validated shear response of 54–74 pC/N in were accompanied by longitudinal responses ranging from 5 to 10 pC/N. Overall, these studies showcase the effectiveness of computational screening and molecular design in steering the discovery of high-performance organic piezoelectrics, bridging the gap between theoretical insights and practical applications in the development of sustainable electromechanical materials.

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