MS14 Materials for energy storage and Conversion

MS14-1-4 Rotationally-driven piezoelectricity: computational assessment of ionic plastic molecular crystals
#MS14-1-4

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Abstract
Piezoelectric materials couple mechanical and electric responses making them suitable for a broad range of applications such as sonar, medical ultrasound, sensors and energy harvesting devices. In this work, we calculate dielectric, piezoelectric and ferroelectric properties of 11 hybrid molecular crystals using van der Waals density functional theory. We predict negative piezoelectric coefficients $d_{33}$ for some of the hybrid molecular crystals. Negative $d_{33}$ values have only been reported earlier for polymers and liquid crystals [1]. Further, the $d_{ij}$s of the hybrid molecular crystals are comparable to phase-pure inorganic piezoelectrics, such as AlN and LiNbO$_3$ see Fig. 1. The computed shear contributions to the piezoelectric response are large, with a $d_{24}$ of -116 pC/N calculated for HdabcoReO$_4$\(^1\). The largest piezoelectric factor of anisotropy |$d_{16}/d_{33}$|=161 for HQReO$_4$\(^2\) is also far larger than for typical inorganic systems such as BaTiO$_3$ with a |$d_{15}/d_{33}$| of 6. We show the large piezoelectric anisotropy can in part be understood from rotations of constituent molecules similar to the polarization vector rotation observed in inorganic perovskites with compositions near to a morphotropic phase boundary [2].

1,4 – diazabicyclo[2.2.2]octane perrhenate
2Quinuclidinium perrhenate

References

The calculated piezoelectric coefficients

![Diagram showing calculated piezoelectric coefficients for hybrid plastic crystals and inorganics.](image-url)