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

E.D. Sødahl [1], J. Walker [2], S. Seyedraoufi [1], C.H. Gørbitz [3], K. Berland [1]
[1]Norwegian University of Life Science - Ås (Norway), [2]Norwegian University of Science and Technology - Trondheim (Norway), [3]University of Oslo - Oslo (Norway)

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

References
[1] I. Urbanaviciute, X. Meng, M. Biler, Y. Wei, T. D. Cornelissen, S. Bhattacharjee, M. Linares, and M. Kemerink, Negative piezoelectric effect in an organic supramolecular ferroelectric, Mater. Horiz. 6, 1688 (2019)
[2] M. Davis, M. Budimir, D. Damjanovic, and N. Setter, Rotator and extender ferroelectrics: Importance of the shear coefficient to the piezoelectric properties of domain- engineered crystals and ceramics, Journal of Applied Physics 101, 054112 (2007), publisher: American Institute of Physics

The calculated piezoelectric coefficients