Density Functional Theory (DFT) : Designing Crystalline Piezoelectrics

GEETU KUMARI[1]

[1]*Department of Physics, University of Limerick, Castletroy, Limerick, Republic of Ireland, V94T9PX*
Geetu.Kumari@ul.ie

Accelerating the identification of a biomolecular crystal with an extraordinarily high piezo response is one of the main objectives of our group's research project Pb-FREE. Crystallizing biomolecules creates a network of unit cell dipoles identical to the mechanisms of classical inorganic piezoelectrics, which allows for biological single crystals to easily fulfil the role of piezoceramics, e.g., in stack actuation. Biomolecular piezoelectric materials are considered a strong candidate material for biomedical applications due to their robust piezoelectricity, biocompatibility, and low dielectric property. A combination of modelling and characterization can provide much-needed insight into how piezoelectric properties are modulated by unit cell properties, such as dipole moments, molecular packing, and composition.
Using automation, computer simulations can make the integration of high throughput screening simpler. We are exploring biomolecular crystals for excellent piezoelectric performance using high throughput Density Functional Theory (DFT) computations. (DFT) utilizes periodic boundary conditions to simulate bulk material behavior and can quantify material physical properties of crystals, including the dielectric, elastic, and piezoelectric constants. By studying biomolecular crystals in this way, the predicted physical properties can be directly related to single crystal experiments, allowing effective screening of organic crystals for experimental investigation. In this talk, I will discuss the piezoelectric properties of a number of novel, multi-component crystals I have screened using these methods.

References:

1. Ibn-Mohammed, T.; Koh, S.; Reaney, I.; Sinclair, D.; Mustapha, K.; Acquaye, A.; Wang, D., Are lead-free piezoelectrics more environmentally friendly? MRS Communications 2017, 7 (1), 1-7.
2. E Kiely, R Zwane, R Fox, AM Reilly, S Guerin., Density functional theory predictions of the mechanical properties of crystalline materials. CrystEngComm, 2021, 23(34), 5697-5710
3. De Jong, M., Chen, W., Geerlings, H., Asta, M., & Persson, K. A. (2015). A database to enable discovery and design of piezoelectric materials. Scientific data, 2(1), 1-13.
4. Guerin, Sarah. "Getting the Lead Out: Biomolecular Crystals as Low-Cost, High-Performance Piezoelectric Components." Accounts of Materials Research 3, no. 8 (2022): 782-784.