Developing a Theory of Molecular Piezoelectricity

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In previous work we have studied the piezoelectricity of organic crystals by exploring the strain of small subsystems in response to an applied field [1]. By reducing the dimensionality of the problem, we were able to establish a simple mathematical model which could be used to predict the piezoelectric coefficient of hydrogen-bonded systems [2]. In the present work we have extended the model to account for the geometric response on the fully-dimensional potential energy surface. We have established a systematic method for predicting the piezoelectric properties of small molecules in the zero-field limit. Furthermore, we have elucidated the deeper connections to strain theory for bulk materials and have developed a formalism for describing the complicated anisotropic piezoelectric response of molecules. We demonstrate that our analytic formalism is consistent with results from numerical studies.

[1] K. A. Werling, G. R. Hutchison, and D. S. Lambrecht, “Piezoelectric Effects of Applied Electric Fields on Hydrogen-Bond Interactions: First-Principles Electronic Structure Investigation of Weak Electrostatic Interactions”, *J. Phys. Chem. Lett.* **4**, 1365-1370 (2013). http://dx.doi.org/10.1021/jz400355v

[2] K. A. Werling, M. Griffin, G. R. Hutchison, and D. S. Lambrecht, "Piezoelectric Hydrogen Bonding: Computational Screening for a Design Rationale", *J. Phys. Chem. A* **118**, 7404-7410 (2014). http://dx.doi.org/10.1021/jp412740j