Accelerated Piezoelectric Evaluation (APE)

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Piezoelectric materials produce an electric charge when mechanically deformed and can be deformed by an electric charge. This dual property can be used to harvest power from movement and provide a shock sensor; uses that range from recharging pacemakers with a heartbeat to firing an airbag when a collision occurs. Normally, piezoelectric materials have been inorganic, but this project looks to investigate organic monomers as they have a different potential set of uses and can more easily be varied. Calculating the coefficient was tedious and time consuming; automating that process opens up the ability to find trends and monomers that give a high piezoelectric response. I created the accelerated piezoelectric evaluator (APE) which is an automated script that uses the coordinates from a dimer system to return a piezoelectric coefficient. This process takes a fraction of the time it takes to do the calculations by hand and is repeatable. APE finds two monomers from the set of coordinates and then distances them from one another along a hydrogen bond between them. It then uses the Q-Chem program package to calculate potential energy curves. From this information, the piezoelectric coefficient along the hydrogen bond axis is calculated via the second derivative and dipole moment. Preliminary results are consistent with previously calculated values and initial tests with a pool of candidates revealed some monomers that have high piezoelectric coefficients. APE can be interfaced with other approaches such as genetic algorithms for new material discovery.