Tailorable Organic Nanoscale Piezoelectrics for Energy Harvesting

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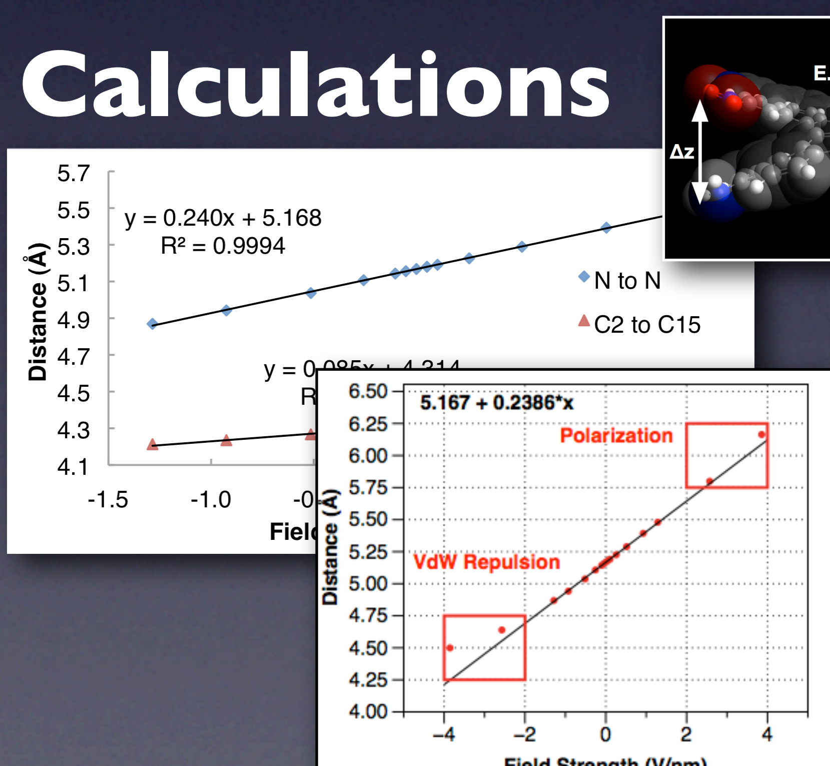
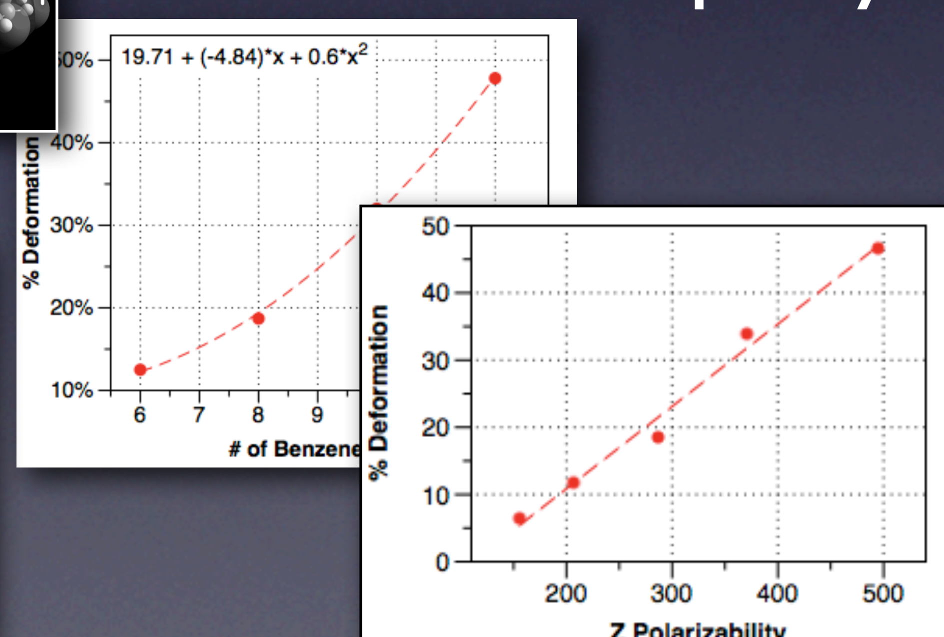
Piezoelectric materials deform their shape in response to an applied electric field or generate electric charge in response to a shape change. We demonstrated via density functional theory (DFT) calculations that polar molecules such as helicenes show immense piezoelectric deformations ~12% of the molecular length (d_{33} = 46 pm/V) much greater than existing polymers such as polyvinyldine difluoride and inorganic materials such as ZnO (d_{33} = -33 pm/V, and 20-30 pm/V, respectively). We used these calculations to derive structure/property relationships, pointing to increased response, up to ~50% deformations with increased polarizability.

We also demonstrated for the first time, the piezoelectric response of **single monolayers** of piezoelectric oligopeptides using piezoresponse atomic force microscopy (Piezo-AFM). Measured response was much greater from piezo-active peptides than from inactive alkanethiols, and in good agreement with computational predictions. We will use both experiment and calculations to drive the design of new, highly active energy harvesting materials.

Calculations



Structure/Property



Experiment

Piezo AFM