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Project Title.

Low Cost and Clean Energy Storage Based on Molecular Ferroelectrics and Antiferroelectrics

Abstract.

The mismatched energy production and generation require energy storage as the buffer [1]. The problem only gets more severe as global energy consumption increases. Among electricity-based energy storage, electrostatic capacitors have the advantage of high charging-discharging speed, i.e., high power density, as well as large number of cycles, which is especially appealing for pulsed energy sources. However, their energy density and cost need to be improved before the large-scale deployment.

In this project, we propose to study recently discovered molecular ferroelectrics and antiferroelectrics as spacer materials in electrostatic capacitors, taking advantage of their low cost, environmental friendliness, and flexibility. In particular, the polycarboxylic acids family (e.g., squaric acid or SA, and croconic acid or CA) exhibit large polarizations on par with that of the inorganic prototype ferroelectric oxide materials BaTiO₃ and Pb(Zr,Ti)O₃ (PZT), suggesting potentially high dielectric constant which is critical for energy storage. The overarching **goal** of this project is to exploit molecular ferroelectric and antiferroelectric films for clean energy storage with high energy density and high power density.

The specific objectives are:

- (1) Prepare film structures of molecular ferroelectric with controlled microstructure and interfaces.
- (2) Determine the effects of microstructures and interfaces on energy-storage related properties such as the dielectric constant and breakdown electric fields, and compare them with the parameters of canonical ferroelectric oxides.
- (3) Elucidate the structural and electronic structural origin of the charging-discharging (polarization switching) processes.

The success of this project will provide guidance for finding low cost and environmentally benign material systems for high power energy storage, fully utilizing the diverse energy sources to cope with the fluctuating energy consumption and increase the resilience of energy infrastructure.