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DESIGNING FLEXOELECTRIC METAMATERIALS THROUGH COMPUTATIONAL STRAIN GRADIENT ENGINEERING

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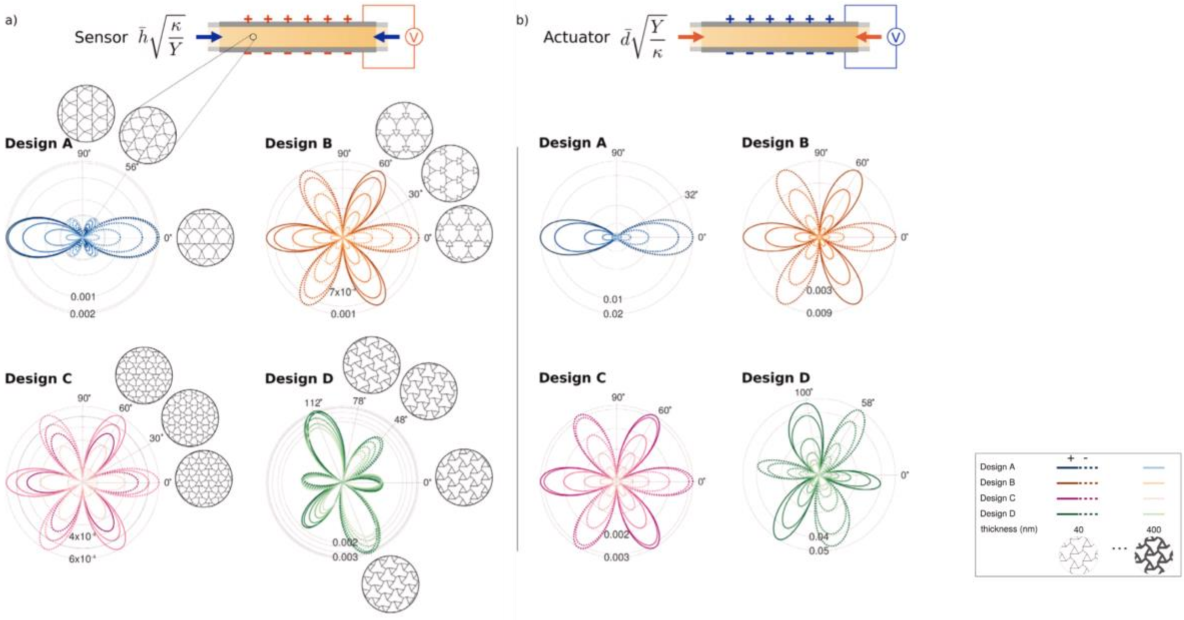
ABSTRACT

It is well known that by deforming some materials (piezoelectrics) electricity can be produced. This functionality makes piezoelectrics ubiquitous in sensors, actuators, and energy harvesting systems. However, only a limited set of materials exhibit piezoelectricity, which limits many technologies. Applying a strain gradient to a dielectric, e.g. by bending, also generates electric fields due to the so-called flexoelectric effect, which conversely generates strains under applied electric field gradients [1]. Unlike piezoelectricity, this effect is universal to all dielectrics, and hence of potential broad applicability. However, flexoelectric electromechanical transduction is significant only at sub-micron scales, where high strain-gradients develop, and for this reason this effect has only been characterized and is being applied in recent years. Unlike piezoelectricity, the interpretation of experiments and the design of functional devices exploiting flexoelectricity requires accurate solutions of coupled electromechanical high-order boundary value problems on complex geometries, since field gradients are required and we lack intuition on such problems.

In this talk, I will present a theoretical and computational framework to solve general flexoelectric boundary value problems based on an Immersed Boundary Hierarchical B-spline approach [2.3]. I will discuss how these calculations allow us to conceive, quantify and optimize a new class of metamaterials and composites that constructively accumulate the flexoelectric effect of nonpiezoelectric micro-structural elements, and make it available as an apparent piezoelectric response at larger scales [4,5]. These multi-scale metamaterials mobilize under homogeneous macroscopic strain substantial strain gradients (and polarization) in its non-piezoelectric constituents, and ensure a buildup of generated field in the material by their non-centrosymmetric arrangement. I will also discuss how large deformations can strongly enhance the flexoelectric effect in soft materials, and furthermore, how buckling-induced emergent geometric polarization can lead to tunable/switchable electromechanical materials, or to the mechanical self-assembly of large-area flexoelectric devices. Finally, I will discuss the connection between continuum theories of flexoelectricity and atomistic models based on electronic structure calculations [6].



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