

## A COMPUTATIONAL STUDY OF FLEXOELECTRICITY IN NANOSTRUCTURES

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**Key words:** *Flexoelectricity, Piezoelectricity, Nanostructures, Computational mechanics, Meshfree methods.*

Flexoelectricity is a size-dependent electromechanical coupling mechanism, existing in a wide variety of materials, including cellular membranes, liquid crystals, carbon-based materials, and piezoelectric and non-piezoelectric crystals. Flexoelectricity manifests noticeably at the nanoscale, therefore experimental observation of this phenomenon is more difficult compared to other electromechanical coupling mechanisms such as piezoelectricity. This motivates us to develop theoretical and computational models to investigate flexoelectricity in nanostructures.

A number of theoretical models have been proposed to understand the flexoelectric behavior of dielectric nanostructures [1, 2]. However, the solutions to these models have been based on atomistic simulations or analytical calculations. The atomistic simulations have been mainly performed to estimate the flexoelectric coefficients and they are limited to small system sizes. On the other hand, in the continuum framework, the governing partial differential equations of flexoelectricity are of fourth order, making the analytical calculation a difficult task. In all cases, simple geometries with simplifying assumptions have been considered to facilitate the calculations. These assumptions may lead to under- or over-estimation of the flexoelectric effect. Furthermore, this effect can be more prominent in complex geometries for which analytical solutions are cumbersome or impossible to obtain. In this work, we employ a mesh-free method based on local maximum-entropy (LME) approximants [3]. Their basis functions exhibit a  $(C^\infty)$  smoothness which allow us to deal with the fourth order terms of the governing equations. We focus on the most commonly used method to quantify the flexoelectric response of nanostructures, which is the bending of a cantilever nano-beam. Figure 1 presents the results of the model. The beam converts the mechanical energy of the applied load  $\mathbf{F}$  to electric potential due to

flexoelectricity. The results show clearly that decreasing the beam thickness leads to a significant enhancement of energy conversion at the nanoscale, in agreement with analytical results. A non-uniform electric potential distribution is also observed along the beam in which the potential difference reaches the maximum value at the left-end support. A similar non-uniform response has been reported experimentally by the local probing of piezoresponse in buckled PZT nano-ribbons [4].

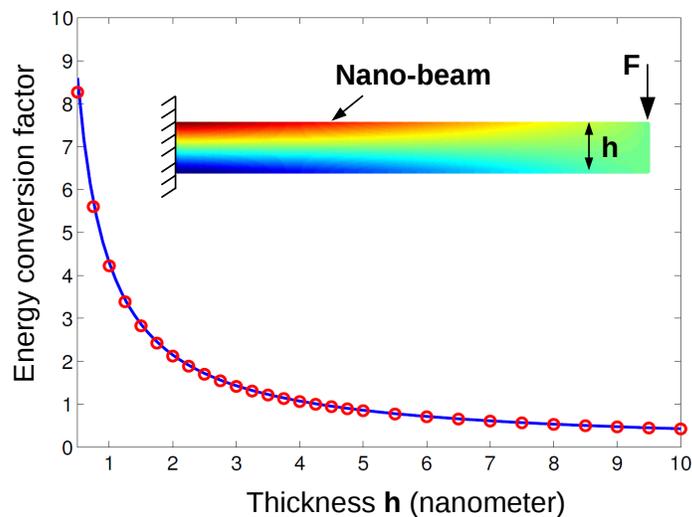


Figure 1: Electromechanical energy conversion factor of a nano-beam as a function of thickness. The color contour indicates the distribution of electric potential. Energy conversion increases significantly by decreasing the beam thickness at the nanoscale.

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