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MATHEMATICAL AND COMPUTATIONAL MODELING OF FLEXOELECTRICITY AT MESOSCOPIC AND ATOMISTIC SCALES

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The presented work [1] has been recently awarded by the Spanish Association for Computational Mechanics and Engineering (SEMNI) as the best 2021 PhD thesis in Spain about numerical methods and related fields.

The topic of the thesis is the development of mathematical and computational models for flexoelectricity, a relatively new electromechanical coupling that is present in any dielectric at the micron and sub-micron scales. The work is framed in the context of both continuum and quantum mechanics, and explores the gap between these two disciplines.

On the one hand, the focus is put on the mathematical modeling of the flexoelectric effect by means of continuum (electro-) mechanics, and the development of computational techniques required to numerically solve the associated boundary value problems. The novel computational infrastructure developed in this work is able to predict the performance of engineered devices for electromechanical transduction at sub-micron scales, where flexoelectricity is always present, without any particular restrictions in geometry, material choice, boundary conditions or nonlinearity. Flexoelectricity can be harnessed in multiple different ways towards the development of breakthrough applications in nanotechnology, as shown by different numerical examples.

On the other hand, the flexoelectric effect is also studied at an atomistic level by means of quantum mechanics. A novel methodology to quantify the flexoelectric properties of dielectric materials is proposed, by means of connecting ab-initio atomistic simulations with the proposed models at a coarser, continuum scales. The developed approach sheds some light on a controversial topic within the density functional theory community, where large disagreements among different theoretical derivations are typically found. The ab-initio computations serve not only to assess the material parameters within the continuum models, but also to validate their inherent assumptions regarding the relevant physics at the nanoscale.

REFERENCES

[1] D. Codony, Mathematical and computational modeling of flexoelectricity at mesoscopic and atomistic scales, TDX (Tesis Doctorals en Xarxa) (2021) Published by Universitat Politècnica de Catalunya. Postprint (published version)