An atomistic model for flexoelectricity tensor in non-perfect graphene

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Abstract

Unlike piezoelectricity, flexoelectricity is a form of electromechanical coupling allowed for crystals with central symmetry in the unit cell. However, flexoelectricity was rarely considered for electromechanical transduction and energy harvesting because of its expected weak impact at macroscopic scales. Nevertheless, recent studies have shown the interest of understanding its intrinsic mechanism at the nanoscale. Meanwhile, lots of progress has been made with respect to 2D materials, such as graphene. For instance, molecular dynamics (MD) simulations have recently been used to shown how flexoelectricity tensor components for graphene can be improved by structuring it[1]. These MD simulations used a charge-dipole model[2-4] that requires solution of a large linear system at each step. In order to improve this approach, we coupled the previous atomistic approach with continuum mechanics through a generalized Cauchy-Born approximation to derive an analytic formula allowing to compute the flexoelectricity tensors directly from the detailed knowledge of the equilibrium state, similarly to what can be done for the evaluation of e.g. elastic moduli. Preliminary results of a comparison between our results and those reported by Javvaji et al. will be presented in the poster.

References

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