# Structural properties and electrical conductivity of electro-responsive polymer nanocomposites through coarse-grained Langevin dynamics.

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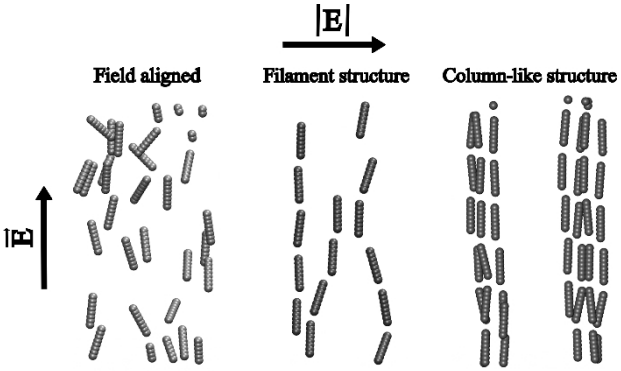
Responsive polymer nanocomposites (PNCs) are a promising class of materials for designing smart systems. In this study, we employ coarse-grained Langevin dynamics to investigate the structural, and electrical properties of a PNC. This nanocomposite is constituted by polarizable nanorods (NRs) embedded within a polymer matrix under direct-current electric fields of varying amplitude. Our results show different structural motifs of the NRs depending on the amplitude of the applied field. At low field amplitudes, the NRs orient along the field direction, whereas at high amplitudes they self-assemble into percolating filaments and column-like structures. To compute the electrical conductivity of the system, we use both a resistor network model [1] and a theoretical model [2] for aligned and unaligned NRs. When comparing both models, the results show a disagreement in the computed electrical conductivity. This occurs because the theoretical model is incapable of accounting for the self-assembly of the NRs. To improve it and account for this self-assembly, we modify one of its parameters, which results in an electrical conductivity similar to that obtained with the resistor network. Therefore, our simulations results suggest that the structural motifs of the NRs directly affects the material's electrical conductivity, with an enhancement of around four orders of magnitude between low and high electric field amplitudes.




*Self-assembled motifs at increasing amplitudes of the applied direct current electric field.*

**References:**

[1] W. S. Bao, S. A. Meguid, Z. H. Zhu, G. J. Weng. Mechanics of Materials, 46, 129-138. 2012.
[2] A.Chanda, S. K. Sinha, N. V. Datla. Composites Part A: Applied Science and Manufacturing, 149, 106543. 2021.

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