# Reactive Molecular Dynamics Applied to the Study of Mechanical Properties of Biphenylene Nanotube

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Recently (2021) a research group published a new synthetic route that resulted in the delivery of a two-dimensional structure similar to graphene: biphenylene (BPN), characterized by the composition of its rings with 4, 6 and 8 atoms [1]. The studies carried out by this group showed that the BPN armchair nanoribbons have electronic properties similar to those of a graphene armchair with the same dimensions. In this sense, the BPN structure in 2D layers appears as a promising material that needs to be investigated in terms of structural, electronic and thermomechanical properties. Even before being synthesized, there were already a considerable amount of publications bringing theoretical results regarding its electronic and structural properties [2]. In this work, we perform fully atomistic molecular dynamics simulations with the ReaxFF reactive force field of the mechanical and thermal properties of an armchair and zig-zag nanotube made of BPN sheets. Despite the properties of this new structure between BPN and graphene, the ones proposed as electronic properties of the new structure are quite metallic, since graphene show opponents. According to the authors' study, the biphenylene lattice bands are only 21 atoms wide and behave as an energy-conducting material. Graphene indicates a semiconductor behavior in the same imposed dimensions [1]. These characteristics make the potential technological applications of biphenylene promising soon, such as the use in conducting wires of electronic devices or even a use of BPN networks as a superior anode in lithium-ion batteries, being able to reach a capacity storage batteries comparable to current graphene-based materials [1].

**Acknowledgment:** The authors gratefully acknowledge the financial support from the Brazilian Research Councils CAPES, CNPq and FAPDF.

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