N-doped graphene: polarization effects and structural properties

Mehdi Neek-Amal[1], H. Ghorbanfekr[2], F. M. Peeters[2]

[1]Department of Physics, Shahid Rajaee Teacher Training University, 16875-163, Lavizan, Tehran, Iran.

[2]Department of Physics, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium.

Structural and mechanical properties of N-doped graphene (NG) are investigated using ReaxFF potentials in large scale molecular dynamics simulations. We found that ripples, which are induced by the dopants, changes the roughness of NG which depend on the number of dopants and their local arrangement. For any doping ratio N/C the NG becomes ferroelectric with a net dipole moment. The formation energy increases non-linearly with N/C ratio, while the Young's modulus, tensile strength and intrinsic strain decreases with the number of dopants. Our results for the structural deformation and the thermo-electricity of the NG sheet are in good agreement with recent experiments and ab-initio calculations.