N-doped graphene: Polarization effects and structural properties

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Abstract

The structural and mechanical properties of N-doped graphene (NG) are investigated using reactive force field (ReaxFF) potentials in large-scale molecular dynamics simulations.We found that ripples, which are induced by the dopants, change the roughness of NG, which depends on the number of dopants and their local arrangement. For any doping ratio N/C, theNGbecomes ferroelectricwith a net dipole moment. The formation energy increases nonlinearly with N/C ratio, while the Young's modulus, tensile strength, and intrinsic strain decrease with the number of dopants. Our results for the structural deformation and the thermoelectricity of the NG sheet are in good agreement with recent experiments and *ab initio* calculation.