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First-principles study of polarization in graphene PRIYAMVADA JADAUN, YUGUI YAO, LEONARD F. REGISTER, QIAN NIU, SANJAY BANERJEE, The University of Texas at Austin — The emergence of polarization in monolayer graphene is investigated using first-principles calculations. We try to understand electronic polarization calculated using Berry phase technique as well as ionic polarization when in-plane symmetry is broken within the graphene lattice. The effect of underlying substrate as well as stress on this symmetry breaking is also explored.

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