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Gap opening in graphene by 1D and 2D periodic corrugations
IVAN NAUMOV, ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories, 1501 Page Mill Road, Palo Alto, California 94304, USA — Using first-principles methods and symmetry arguments, we show that a graphene monolayer, which is periodically corrugated in one or two direction(s), can be either semimetal or semiconductor, depending on how strong corrugation is or how the initial symmetry is broken. In the case of 1D periodic ripples, a gap at the Dirac points opens up only due to (i) breaking of the inversion symmetry or equivalence between A and B sublattices and/or (ii) merging of two inequivalent Dirac points, **D** and -**D**. Since breaking the inversion symmetry has only relatively modest effect, a tangible gap can be mainly induced by mutual annihilation of the Dirac points, which requires large corrugations, close to mechanical breaking point. In contrast to 1D, the 2D ripples can additionally induce a semiconducting gap via mixing of electronic states belonging to two different **K**, **K′** valleys. In this case, a gap on the order of 0.5 eV can be opened up at strains safely lower than the graphene failure strain [1].

[1] I.I. Naumov, A.M. Bratkovsky, arXiv:1104.0314v1.

Ivan Naumov
Hewlett-Packard Laboratories, 1501 Page Mill Road,
Palo Alto, California 94304, USA

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