Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

One Dimensional Massless Dirac Fermions in Functionalized Graphene Nanoribbons

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— Low-energy excitations of graphene are massless Dirac fermions due to presence of linear bands crossing at the Fermi level. Zigzag-edged nanoribbons of graphene (ZGNR), however, being semiconducting, do not possess this property. Using ab initio density-functional theory calculations we find that it is possible to close the band gap of ZGNRs through edge-functionalization with Na atoms. Moreover, the resulting band structure displays tilted-v-shaped linear bands crossing at the Fermi level, corresponding to one-dimensional massless Dirac fermions. We discuss mechanism of formation of such a band structure and its consequences in terms of electronic and transport properties.

1Supported by TÜBİTAK, Project No: 111T318

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Date submitted: 09 Nov 2011

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