

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Highly anisotropic Dirac fermions in square graphynes LIZHI ZHANG, Univ of Electronic Sci Tech / University of Utah, ZHENGFEEI WANG, University of Science and Technology of China, JIANSHEG RAO, ZIHENG LI, WULIN HUANG, ZHIMING WANG, Univ of Electronic Sci Tech, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, FENG LIU, University of Utah — Recently, there have been intense search of new 2D materials, and one especially appealing class of 2D materials is the all-carbon allotropes of Dirac materials. Here, we predict a new family of 2D carbon allotropes, square graphynes (S-graphynes) that exhibit highly anisotropic Dirac Fermions, using first-principle calculations within density functional theory. The equal-energy contour of their 3D band structure shows a crescent shape, and the Dirac crescent has varying Fermi velocities from $0.6 \cdot 10^5$ to $7.2 \cdot 10^5$ m/s along different k directions. Near the Fermi level, the Dirac crescent can be nicely expressed by an extended 2D Dirac model Hamiltonian. Furthermore, tight-binding band fitting reveals that the Dirac crescent originates from the next-nearest-neighbor interactions between C atoms. Our findings enrich the Dirac physics founded in other 2D Dirac systems, and offer a new design mechanism for creating Dirac band by tuning the interaction range. We envision that the highly anisotropic Dirac crescent may be exploited in all-carbon-based electronic devices for manipulating anisotropic electron propagation.

Lizhi Zhang
Univ of Electronic Sci
Tech

Date submitted: 28 Jan 2016

Electronic form version 1.4