COLLOQUIUM (2016-2)

School of Materials Science & Engineering

"Dirac semimetal properties of black phosphorus"

Prof. Choi, Hyoung Joon

(Dept. of Physics, Yonsei Univ.)

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APRI 1F, Auditorium Hall

Dirac semimetal properties of black phosphorus

Hyoung Joon Choi
Department of Physics, Yonsei University, Seoul, Korea

Thin flakes of black phosphorus (BP) are a two-dimensional (2D) semiconductor whose energy gap is predicted being sensitive to the number of layers and external perturbations. Very recently, it was found that a simple method of potassium (K) doping on the surface of BP closes its band gap completely, producing a Dirac semimetal state with a linear band dispersion in the armchair direction and a quadratic one in the zigzag direction [1]. Here, based on first-principles density functional calculations, we predict that beyond the critical K density of the gap closure, 2D massless Dirac fermions (i.e. Dirac cones) emerge in K-doped few-layer BP, with linear band dispersions in all momentum directions, and the electronic states around Dirac points have chiral pseudospins and Berry's phase [2]. These features are robust with respect to the spin-orbit interaction and may lead to graphene-like electronic transport properties with greater flexibility for potential device applications.

[1] J. Kim, S. S. Baik, S. H. Ryu, Y. Sohn, S. Park, B.-G. Park, J. Denlinger, Y. Yi, H. J. Choi, and K. S. Kim, Science **349**, 723 (2015)

[2] S. S. Baik, K. S. Kim, Y. Yi, and H. J. Choi, Nano Letters **15**, 7788 (2015)

Hyoung Joon Choi

Professor, Department of Physics, Yonsei University

Address: 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Republic of Korea
Telephone: (82)2-2123-2608 **Fax:** (82)2-392-1592
E-mail: h.j.choi@yonsei.ac.kr **Nationality:** Republic of Korea
Web: http://web.yonsei.ac.kr/choi

EDUCATION

Seoul National University	Ph.D	Physics	**2000**
Seoul National University	MS	Physics	**1994**
Seoul National University	BS	Physics	**1992**

PROFESSIONAL ACTIVITIES

- Professor, Department of Physics, Yonsei University, Seoul, Korea (2005 to Present)
- Director, Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University (2011 to Present)
- Fellow, The Korean Physical Society (2011 to Present)
- Professor, Korea Institute for Advanced Study, Seoul, Korea (2003 to 2005)
- Miller Research Fellow, University of California, Berkeley, CA, USA (2000 to 2003)

RESEARCH INTERESTS

- First-principles study of electronic transport in nanostructures: carbon nanotubes, molecular electronic devices, magnetic tunnel junctions, graphene nanoribbons, semiconductor nanostructures, and oxide nanostructures
- Ab-initio calculation of electronic, magnetic, and phononic properties of materials: Sr_2RuO_4, copper oxides, iron pnictides, iron chalcogenides, C_{60}, carbon nanotube, graphene, graphite, Si surface, topological insulators, and metal oxides
- Theoretical investigation of superconducting properties: MgB_2, FeAs-based superconductors, and high-T_c copper oxide superconductors.
- Development of computational methods: electronic transport in nanostructures, superconductivity, LSDA+U methods, noncollinear-spin calculations, spin-orbit coupling, and many-body effects.

SELECTED PUBLICATION

- Observation of tunable band gap and anisotropic Dirac semimetal state in black phosphorus. J. Kim, S. S. Baik, S. H. Ryu, Y. Sohn, S. Park, B.-G. Park, J. Denlinger, Y. Yi, H. J. Choi, and K. S. Kim, Science **349**, 723 (2015)
- Emergence of two-dimensional massless Dirac Fermions, chiral pseudospins, and Berry's phase in potassium doped few-layer black phosphorus. S. S. Baik, K. S. Kim, Y. Yi, and H. J. Choi, Nano Letters **15**, 7788 (2015)
- The origin of the anomalous superconducting properties of MgB_2. H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, and S. G. Louie, Nature **418**, 758 (2002).
- Broken symmetry and pseudogaps in ropes of carbon nanotubes. P. Delaney, H. J. Choi, J. Ihm, S. G. Louie, and M. L. Cohen, Nature **391**, 466 (1998).

- Crossed nanotube junctions. M. S. Fuhrer, J. Nygard, L. Shih, M. Forero, Y.-G. Yoon, M. S. C. Mazzoni, H. J. Choi, J. Ihm, S. G. Louie, A. Zettl, and P. L. McEuen, Science **288**, 494 (2000).
- Band structure and Fermi surface of electron-doped C_{60} monolayers. W. L. Yang, V. Brouet, X. J. Zhou, H. J. Choi, S. G. Louie, M. L. Cohen, S. A. Kellar, P. V. Bogdanov, A. Lanzara, A. Goldoni, F. Parmigiani, Z. Hussain, and Z.-X. Shen, Science **300**, 303 (2003).
- Mechanically-controlled binary conductance switching of a single-molecule junction. S. Y. Quek, M. Kamenetska, M. L. Steigerwald, H. J. Choi, S. G. Louie, M. S. Hybertsen, J. B. Neaton, and L. Venkataraman, Nature Nanotechnology **4**, 230 (2009).
- Time-resolved energy transduction in a quantum capacitor. W. Jung, D. Cho, M.-K. Kim, H. J. Choi, and I.-W. Lyo, PNAS **108**, 13973 (2011).
- Defects, quasibound states, and quantum conductance in metallic carbon nanotubes. H. J. Choi, J. Ihm, S. G. Louie, and M. L. Cohen, Physical Review Letters **84**, 2917 (2000).
- Electrical switching in metallic carbon nanotubes. Y.-W. Son, J. Ihm, M. L. Cohen, S. G. Louie, and H. J. Choi, Physical Review Letters **95**, 216602 (2005).
- Origin of anomalous electronic structures of epitaxial graphene on silicon carbide. S. Kim, J. Ihm, H. J. Choi, and Y.-W. Son, Physical Review Letters **100**, 176802 (2008).
- Chalcogen-height dependent magnetic interactions and magnetic order switching in $FeSe_xTe_{1-x}$. C.-Y. Moon and H. J. Choi, Physical Review Letters **104**, 057003 (2010).
- Single-impurity scattering and carrier mobility in doped Ge/Si core-shell nanowires. H. Lee and H. J. Choi, Nano Letters **10**, 2207 (2010).
- Nanometer-scale loop currents and induced magnetic dipoles in carbon nanotubes with defects. J. Im, Y. Kim, C.-K. Lee, M. Kim, J. Ihm, and H. J. Choi, Nano Letters **11**, 1418 (2011).