Highlights

Superconductivity - 2016

First-principles and angle-resolved photoemission study of lithium doped metallic black phosphorous

A. Sanna[1], A.V. Federov[2,3,4], N. I. Verbitskiy[2,5,6], J. Fink[3], C. Krellner[7], L. Petaccia[8], A. Chikina[9,4], D. Yu Usachov[4], A. Grüneis and G. Profeta[10]

[1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany
[2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany
[3]IFW Dresden, PO Box 270116, D-01171 Dresden, Germany
[4]St. Petersburg State University, St. Petersburg, 198504, Russia
[5]Faculty of Physics, University of Vienna, Strudlhofgasse 4, A-1090 Vienna, Austria
[6]Department of Materials Science, Moscow State University, Leninskiye Gory 1/3, 119992, Moscow, Russia
[7]Physikalisches Institut, Goethe-Universität Frankfurt, Max-von-Laue- Straße 1, D-60438 Frankfurt am Main, Germany
[8]Elettra Sincrotrone Trieste, Strata Statale 14 km 163,5, I-34149 Trieste, Italy
[9]Institute of Solid State Physics, Dresden University of Technology, Zellescher Weg 16, D-01062 Dresden, Germany
[10]Department of Physical and Chemical Sciences and SPIN-CNR, University of L'Aquila, Via Vetoio 10, 67100 L'Aquila, Italy

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First principles calculations demonstrate the metallization of phosphorene by means of Li doping filling the unoccupied antibonding *p z* states. The electron-phonon coupling in the metallic phase is strong enough to eventually lead to a superconducting phase at *Tc* = 17 K for LiP_8 stoichiometry. Using angle-resolved photoemission spectroscopy we confirm that the surface of black phosphorus can be chemically functionalized using Li atoms which donate their 2s electron to the conduction band. The combined theoretical and experimental study demonstrates the semiconductor-metal transition indicating a feasible way to induce a superconducting phase in phosphorene and few-layer black phosphorus.

The theoretical predictions of sizable electron-phonon coupling and superconducting phase at 17 K in lithium doped black phosphorus's surface or phosphorene, and its demonstrated experimental feasibility deserves further dedicated studies, already performed on other 2D systems, like four-point probe electrical transport measurements to confirm the existence of a superconducting phase in phosphorene.