Master's thesis project on
Computational Condensed Matter Physics:

Metal to semiconducting phosphorene on curved copper: computer simulations to solve the puzzle

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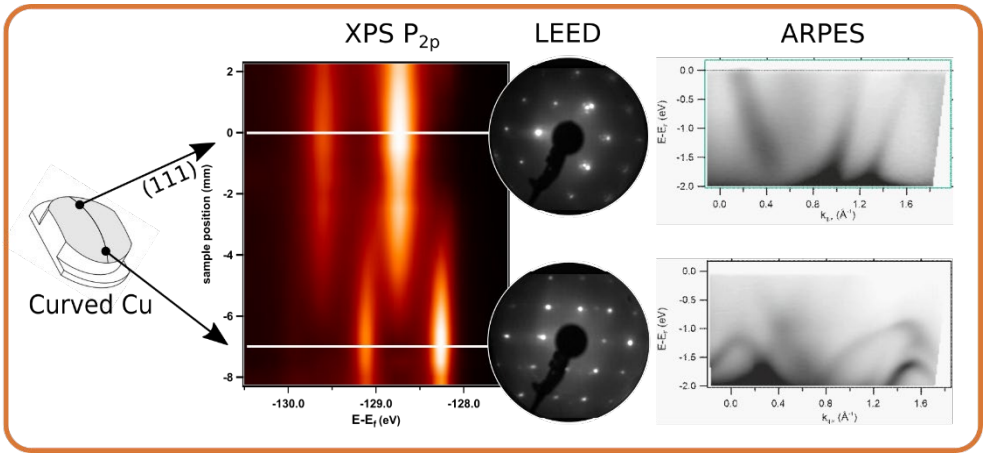
2010 Nobel Prize in Physics was assigned for "*groundbreaking experiments regarding the two-dimensional material graphene*", the latter being isolated in 2004 by Geim and Novoselov. Starting from that moment, the research about 2D materials beyond graphene have experienced a tremendous boost, being also supported by the green technologies increasing demand. In this context, phosphorene, a single layer of black phosphorus, shows great electronic properties, for example the direct band-gap tuneable by the number of layers, that make this material one of the most compelling and studied [1].

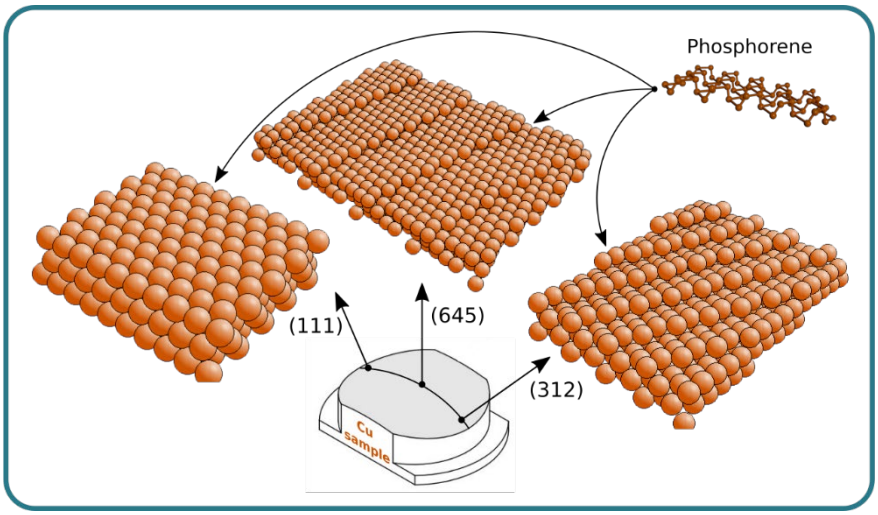


Our experimental collaborators are able to grow a monolayer of phosphorus on a curved single crystal of copper. The substrate spans over a range of crystallographic directions, vicinal to (111), giving phosphorus the possibility "to find" its optimal substrate in which it may reconstruct as a stable 2D layer. There is evidence that, on the same crystal, two diverse phosphorus reconstructions are stable. One of those matches with the blue-phosphorene structure [2] while the other phase has no correspondence in the literature.

Low-Energy Electron Diffraction (LEED) points out that the two reconstructions have a different unit cell, while X-Ray Photoemission Spectroscopy (XPS) shows that they additionally have different chemical environments. Most interestingly, the two phosphorus monolayers exhibit a different electronic behaviour, being one metallic and the other semiconducting, as can be seen from the Angle-Resolved Photoemission Spectroscopy (ARPES) spectra below.

Despite the experimental evidence, “there is plenty of room at the bottom” (R. Feynman) to solve the puzzle and to understand at the atomistic level the peculiar features of one or the other phosphorus structure and the role of the support in its formation.

The work needs therefore a theoretical counterpart, that we envisage should greatly benefit from a twofold approach. The Master’s thesis project will focus on ab-initio density functional theory calculations to be performed using the Quantum ESPRESSO suite of codes [3] on phosphorus structures optimized on different Cu flat surfaces mimicking the possible facets of a curved sample (see Figure above). Beside the optimization of the structures, this study will include their characterization in terms of electronic structure to compare the results with the experimental data mentioned above. On the other side, starting from these and other structures, other collaborators of the Computational Material Science group of the Physics Department will develop machine-trained neural network interatomic potentials to perform molecular dynamics calculations on much larger and more realistic configurations, really mimicking the curved substrate and letting phosphorus to adapt to the different exposed facets. The proponents have already experience on blue phosphorene on gold surfaces [4] and the project on machine trained potential is already in progress. Therefore, the Master’s thesis project will benefit from a close synergy with complementary computational efforts and new exciting experiments and will provide the opportunity to have access to high performance computing resources.



[1] M. Akhtar et al., *Recent advances in synthesis, properties, and applications of phosphorene*, npj 2D Mater. Appl. **1**, 5 (2017).

[2] Y. Kaddar et al., *Dirac Fermions in Blue Phosphorene Monolayer*, Adv. Funct. Mater. **33**, 2213664 (2023).

[3] P. Giannozzi et al., QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials, J.Phys.: Condens. Matter **21**, 395502 (2009).

[4] S. Del Puppo et al., *Blue Phosphorene on Au(111): theory, spectroscopy and diffraction reveal the role of single Au adatoms,* under review in Nanoscale Advances

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