Quantum size effects and electron-phonon coupling in exfoliated black phosphorus and black arsenic

Florian Margot,[1] Simone Lisi,[1] Irène Cucchi,[1] Edoardo Cappelli,[1] Andrew Hunter,[1] Ignacio Gutiérrez-Lezama,[1,2] KeYuhan Ma,[3] Fabian von Rohr,[3,4] Christophe Berthod,[1] Marco Gibertini,[5] Samuel Poncé,[6] Nicolas Marzari,[6] Anna Tamai,[1] Alberto Morpurgo,[1,2] and Felix Baumberger[1,7]

[1] *Department of Quantum Matter Physics, University of Geneva, 24 quai Ernest Ansermet, CH-1211 Geneva, Switzerland*
[2] *Group of Applied Physics, University of Geneva, 24 quai Ernest Ansermet, CH-1211 Geneva, Switzerland*
[3] *Department of Chemistry, University of Zürich, CH-8057 Zürich, Switzerland*
[4] *Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland*
[5] *Dipartimento di Scienze Fisiche, University of Modena and Reggio Emilia, Modena, Emilia-Romagna, Italy*
[6] *Laboratory of theory and simulation of materials, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland*
[7] *Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland*

Quantum confinement profoundly affects the electronic structure of 2D materials as their thickness is reduced down to the atomic limit. Prominent examples include the transition from an indirect to a direct bandgap in transition metal dichalcogenides and the marked increase of the band gap in black phosphorus (BP). Here we present direct measurements of quantum size effects in black phosphorus and black arsenic (BAs), topical 2D semiconductors characterized by a puckered honeycomb crystal structure. Both of these semiconductors offer promising electronic and optoelectronic properties for applications, primarily due to their direct gap and high mobility. Our ARPES measurements map the quantum well state (QWS) dispersion in the valence band of few layer BP and BA. This is achieved by fabricating multiple devices with exfoliated flakes of 2–9 layers thickness encapsulated between graphene and graphite. Based on these measurements, we quantify the anisotropy of the valence band edge and we determine the splitting of the QWS. We find that the splittings differ markedly from the picture of a particle in a box that is used for conventional semiconductor quantum wells (GaAs, Si), but are well described by a tight-binding model. Our ARPES spectra also reveal distinct signatures of electron-phonon coupling, a phenomenon that remained elusive in previous ARPES studies of exfoliated 2D semiconductors but plays a crucial role in the transport properties at elevated temperature.