Brillouin-zone-selection effects in angle-resolved photoemission spectroscopy of silicon

N.R.S. van Venrooij[1,2], Procopios Constantinou*[2,3,4], Taylor J. Z. Stock[2,5], Eleanor Crane[2,5], Alexander Kölker[2,5], Marcel van Loon[2,3], Vladimir N. Strocov[4], Gabriel Aeppli[5,6,7,8], Neil J. Curson[2,5], Steven R. Schofield†[2,3], Michael E. Flatté[1,9]

[1] Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, US

[2] London Centre for Nanotechnology, UCL, WC1H 0AH, London, UK

[3] Department of Physics and Astronomy, UCL, WC1E 6BT, London, UK

[4] Photon Science Division, Paul Scherrer Institute, 5232 Villigen, Switzerland

[5] Department of Electronic and Electrical Engineering, UCL, WC1E 7JE, London, UK

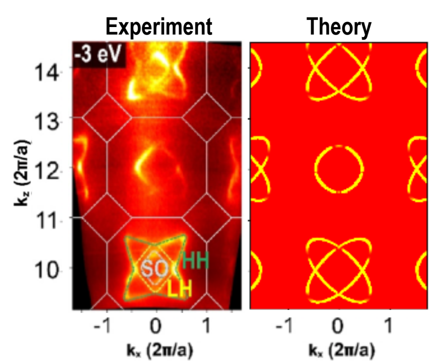
[6] Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne

[7] Department of Physics, ETH Zürich, 8093 Zürich, Switzerland

[8] Quantum Center, ETH Zürich, 8093 Zurich, Switzerland

[9] Department of Applied Physics, Eindhoven University of Technology, Eindhoven 5612 AZ, The Netherlands

The advancement of semiconductor-based atomic-scale quantum electronics hinges on a deep understanding of the electronic properties of subsurface δ-layers[1]. In this rapidly evolving field, soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES) has emerged as a pivotal, non-destructive probing tool[2]. The large energy range of SX-ARPES allows for measurements across a broad momentum space, covering multiple Brillouin zones. During these measurements, interference effects from photoemission across different atoms in a unit cell can lead to pronounced intensity fluctuations between adjacent Brillouin zones, even causing some bands to vanish. In this study, we present the first detailed observations of such photoemission structure factor effects from a cubic semiconductor, revealing periodic fluctuations in both the valence and conduction band states of δ-doped silicon. By applying a simple tight binding calculation to Fermi's golden rule we are able to calculate the structure factor of Silicon and reproduce our experimental findings with a minimal number of approximations. Our findings pave the way for investigations at higher photon energies in the hard X-ray domain, crucial for exploring deeper δ-layers (~10 nm) typical in silicon quantum electronic devices.

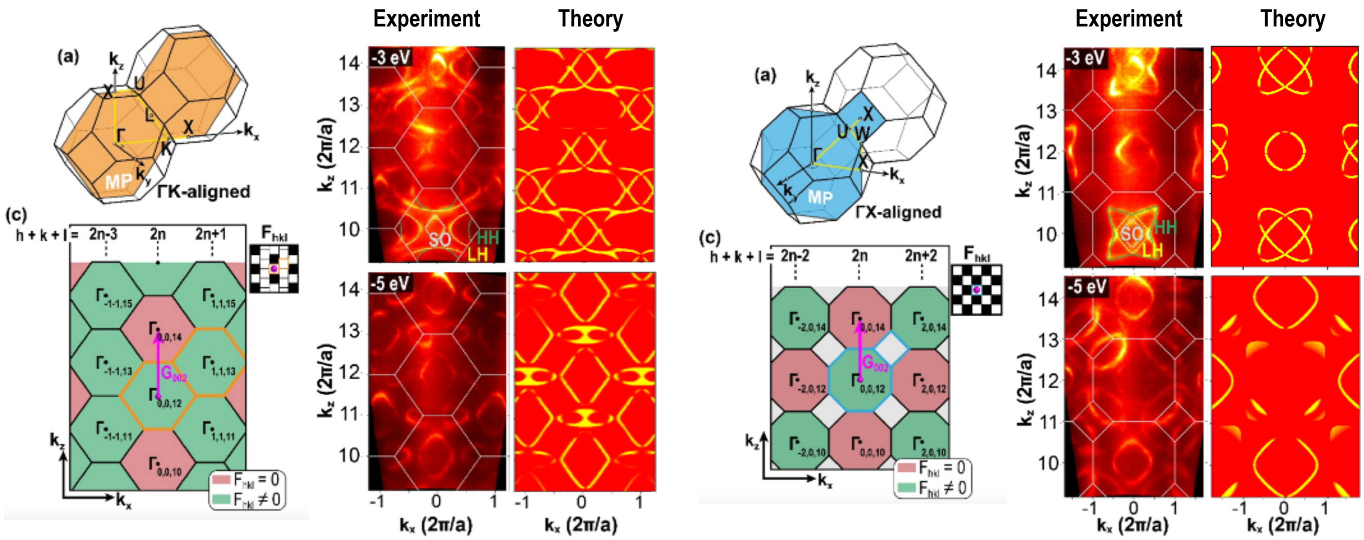


We acknowledge support from the Air Forces Office of Scientific Research (AFOSR), the Engineering and Physical Sciences Research Council (EPSRC) project EP/M009564/1, the EPSRC Centre for Doctoral Training in Advanced Characterisation of Materials (EP/L015277/1), the Paul Scherrer Institute (PSI) and the European Union Horizon 2020 Research and Innovation Program, within the Hidden, Entangled and Resonating Order (HERO) project (810451). Procopios Constantinou was partially supported by Microsoft Corporation.

[1] J. G. Keizer, S. Koelling, P. M. Koenraad, and M. Y. Simmons, "Suppressing Segregation in Highly Phosphorus Doped Silicon Monolayers," *ACS Nano*, vol. 9, no. 12, pp. 12537–12541, 2015, doi: 10.1021/acsnano.5b06299.

[2] V. N. Strocov *et al.*, "Soft-X-ray ARPES at the Swiss Light Source: From 3D Materials to Buried Interfaces and Impurities," *Synchrotron Radiat News*, vol. 27, no. 2, pp. 31–40, 2014, doi: 10.1080/08940886.2014.889550.

Supplementary



The above figure shows the comparison between the ARPES experiment and calculation along two different k-space slices through the Brillouin zone. The theoretical model is successfully able to reproduce different features of the Silicon band structure including the distinctive "checkerboard" patterns.