Band Tuned Enhanced Photodetection in 2D $CuInP_2Se_6$ Interfaced Silicene for NIR photodetectors

Amutha Subramani, Luxa Jan, Kalyan Jyoti Sarkar, Sedmidubsky David, * and Zdeněk Sofer*
The University of Chemistry and Technology, Technická 5, 160 00 Praha 6-Dejvice
subramaa@vscht.cz

Abstract

Photodetectors used in current electronic devices to convert optical impulses into electrical signals, have recently been explored for NIR variations [1-2]. Combination of unique narrow-bandgap electronic and optical properties, along with van der Waals (vdW) surface in 2D materials makes them valuable for advancing the capabilities of non-linear near-infrared (NIR) photodetectors. Emerging 2D van der Waals materials have gained additional interest to develop devices with an improved performance, paving the way for innovations in optoelectronics and information technologies. Here, we use first-principles calculations to examine the structural, electronic, and vibrational features of the as-synthesized 2D non-centrosymmetric van der Waals material, $CuInP_2Se_6$. The study comprehensively investigates various phases, encompassing 2D bulk paraelectric, ferroelectric, and paraelectric monolayer configurations of $CuInP_2Se_6$. Notably, the narrow energy band spectra of $CuInP_2Se_6$ exhibit tunability through phase transitions and layer thickness. The results imply that the paraelectric monolayer phase not only displays a notable response in second harmonic generation (SHG) but also demonstrates lower thermal conductivity, suggesting promising applications in nonlinear optics. Near-infrared silicon photodetectors based on two-dimensional paraelectric monolayer $CuInP_2Se_6$ material with suitable interfacial encapsulation layer is relatively a new design. Furthermore, ab-initio simulations of monolayer silicene demonstrated the appearance of linear band dispersion in planar and low buckling structures of silicene that was stable [3], used here as an encapsulating layer. The designed Au/ $CuInP_2Se_6$/Silicene/SiO_2 photodevice for NIR applications exhibited a significant increase in photoconductive gain due to highly efficient pathway for photocarriers as well as an interfacial encapsulation layer. The optoelectronic device studied using a finite element method had a maximum photoresponsivity of 0.23 A/W at 760 nm. This research reveals the potential to revolutionize integrated nano NIR optoelectronic devices, leading the way for future developments.

References

[1] Y. L. Wu, K. Fukuda, T. Yokota and T. Someya, A Highly Responsive Organic Image Sensor Based on a Two-Terminal Organic Photodetector with Photomultiplication, Adv. Mater. 31 (2019) 1903687.
[2] Y. Wang, J. Kublitski, S. Xing, F. Dollinger, D. Spoltore, J. Benduhn and K. Leo, Narrowband organic photodetectors – towards miniaturized, spectroscopic sensing, Mater. Horiz. 9 (2022) 220-251.
[3] N.J. Roome and J. David Carey Beyond Graphene: Stable Elemental Monolayers of Silicene and Germanene, *ACS* Applied Materials & Interfaces 6 (2014) 7743-7750.

Figures

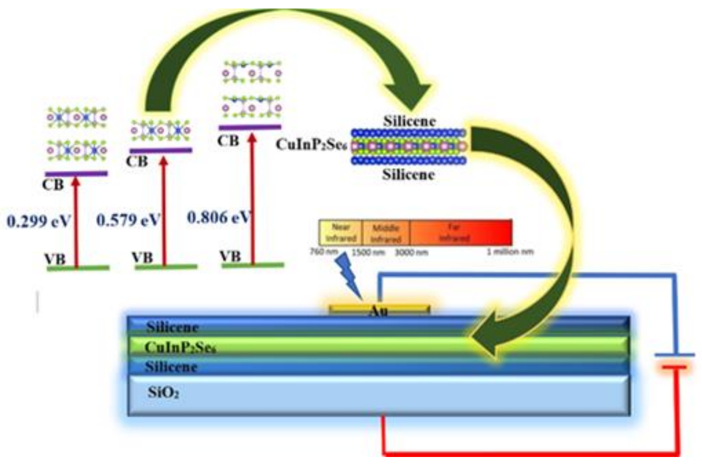

Figure 1: Schematics of the NIR Photodetector employing silicene, $CuInP_2Se_6$, and SiO_2