

## ABSTRACT

## 2D Material as Arsenene 3D Material as CsSbBr<sub>3</sub> Perovskite

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Two dimensional (2D) arsenene, a new allotropic form of arsenene with  $\sqrt{3} \times \sqrt{3} R30^\circ$  reconstruction, exhibiting electronic structure with metallic character, has been revealed on single crystal Ag(111)1 × 1 at temperature of ~ 450 °C, whereas the 2D arsenene with 5 × 5 reconstruction, produces its appearance at a significantly lower temperature of ~ 350 °C. Interesting enough, it was discovered a reversible structural phase transition between these two surface reconstructions, under applying temperature, and/or electron gun irradiation, as established by Auger electron spectroscopy (AES), electron energy diffraction (LEED), and first-principle calculations, by using density functional theory, explicating both atomic structures and their associated band dispersions (ARPES) [1].

Furthermore, staying within the realm of 2D materials, the evidence of  $sp^2$ -like hybridization of silicon valence orbitals in thin-and-thick Si grown on  $\alpha$ -phase Si(111) $\sqrt{3} \times \sqrt{3}R30^\circ$  Bi [2] was, recently, achieved. Instead, just 2D Si(111) islands, on  $\beta$ -phase Si(111) $\sqrt{3} \times \sqrt{3}R30^\circ$ -Bi interface [3] were accomplished. However, moving towards extremely ordered 3D materials, the role of SiO<sub>2</sub> buffer layer in the molecular beam epitaxy growth of CsPbBr<sub>3</sub> perovskite on Si(111), will be also presented [4, 5].

[1] P. De Padova, C. Ottaviani, B. Olivieri and M. Krawiec, 2D Mater., 12 (2025) 025018.

[2] D. Garagnani, et al., Materials 2022, 15, 1730. https://doi.org/10.3390/ma15051730.

[3] P. De Padova, M. Jałochowski, A. Generosi, C. Ottaviani, C. Quaresima, B. Paci, B. Olivieri, M. Krawiec, Microstructure 2024;4:2024019, DOI:10.20517 /microstructure.2023.74.

[4] P. De Padova, et al., Scientific Reports | (2024) 14:23618.

[5] C. Tantardini, et al., J. Phys. Chem. Lett. 2025, 16, 2385.