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ABSTRACT:

Engineering Low-Dimensional Carbon and Phosphorus Structures at Surfaces

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Monoelemental Xenes such as graphene or phosphorene can typically be synthesized via molecular beam epitaxy (MBE) on noble metal substrates like Au(111) and Cu(111). However, the local bonding environment and hybridization with the substrate strongly influence the resulting blue phosphorus (BlueP) structure, often leading to the coexistence of multiple phases and even potential alloy formation. To address this complexity, we introduce a general methodology that combines non-contact atomic force microscopy (nc-AFM) with force spectroscopy [1], enabling the unambiguous discrimination between competing structural models of BlueP/Au(111) derived from density functional theory (DFT). Each BlueP phase is resolved through nc-AFM imaging, while site-dependent force spectroscopy probes local atomic corrugations within the structure. Comparison with probe-particle simulations based on DFT-relaxed geometries reveals that all observed BlueP/Au(111) phases consist of assemblies of $BlueP_9$ or $BlueP_{16}$ units stabilized by Au adatoms.

As a second example [2], we investigate the synthesis of Kagome graphene via on-surface reactions of tribromotrioxoazatriangulene molecules on Au(111). Zero-energy states are subsequently introduced by inserting π-radicals at selected locations within the structure through in situ exposure to atomic hydrogen. nc-AFM imaging and tunneling spectroscopy reveal the stepwise chemical transformation of carbonyl groups into radical species, generating local magnetic defects with spin state S = 1/2 and associated zero-energy states, in agreement with density functional theory calculations.

[1] O. Chahib et al. ACS Nano, in review (2026).
[2] R. Pawlak et al. ACS Nano, 19, 4768–4777 (2025).