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ABSTRACT:

Structure of Atomically-Precise Graphene and Silicene Characterized by Low Temperature Atomic Force Microscopy

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The atomic buckling in 2D “Xenes” (such as graphene, silicene, phosphorene and others) fosters a plethora of exotic electronic properties such as a quantum spin Hall effect which could be engineered by external strain. Quantifying the buckling magnitude with sub-angstrom precision is, however, challenging, since epitaxially grown 2D layers exhibit complex restructurings coexisting on the surface. In this contribution, I will show how we characterized using low-temperature (4,8 K) atomic force microscopy (AFM) with CO-terminated tips assisted by density functional theory (DFT) the structure and local symmetry of prototypical silicene phases on Ag(111) as well as extended defects. Using force spectroscopy, we directly quantify the atomic buckling of these phases within 0.1-Å precision, obtaining corrugations in the 0.8 to 1.1 Å range [1]. The derived band structures further confirm the absence of Dirac cones in any of the silicene phases due to the strong Ag-Si hybridization. I will also discuss our recent works tackling phosphorene structures on gold substrate where the atomic buckling is much larger (3 Å range) [2] as compared to graphene [3] or silicene. Our method paves the way for future atomic-scale analysis of the interplay between structural and electronic properties in other emerging 2D Xenes.

[1] R. Pawlak, C. Drechsel, P. D’Astolfo, M. Kisiel, E. Meyer, J. I. Cerda. Proceedings of the National Academy of Sciences 117, 228-237 (2019).
[2] O. Chahib, J.C. Liu, C. Li, M. Ondracek, P. Jelinek, E. Meyer. In preparation.
[3] R. Pawlak, X. Liu, S. Ninova, P. D’Astolfo, C. Drechsel, S. Sangtarash, R. Häner, S. Decurtins, H. Sadeghi, C. J. Lambert, U. Aschauer, S.-X. Liu, E. Meyer. J. Am. Chem. Soc. 142, 12568-12573 (2020).