Intercalant-induced Kekulé ordering and gap opening in quasi-free-standing graphene

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Abstract
Intercalation of metals at the buffer layer/SiC interface is an effective route to decouple it from the substrate while tailoring its electronic properties. In this work, we investigate the Sn-intercalated buffer layer using low-temperature STM/STS, supplemented by SPA-LEED, and DFT calculations. Sn intercalation effectively decouples the buffer layer, yielding quasi–free-standing monolayer graphene while introducing local lattice distortions. Bias-dependent STM imaging revealed the coexistence of conventional and Kekulé-ordered graphene domains, governed by the underlying Sn(1x1) reconstruction at the SiC interface. The measured STS spectra exhibit good agreement with DFT results. However, achieving homogeneous Sn(1x1) domains remains challenging, apparently, due to strain within the Sn monolayer, which drives the emergence of Kekulé-O distortions and the associated electronic bandgap opening homogeneously in graphene [1]. These findings highlight the crucial role of intercalant homogeneity and strain in tuning graphene's structural and electronic properties.

References

[1] H. T. Ngo, Z. Mamiyev, N. Witt, T. Wehling, and C. Tegenkamp, "Intercalant-induced Kekule ordering and gap opening in quasifreestanding graphene," *Phys. Rev. B*, Feb. 2026, doi: 10.1103/ktj3-t5qk.

Figures

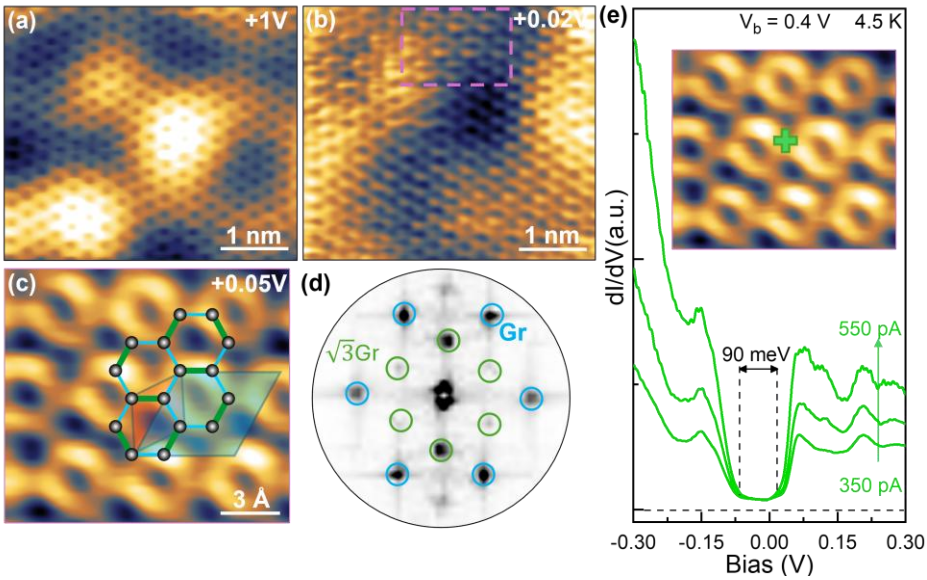

Figure 1: STM topography of a Sn-intercalated BL region measured at (a)+1V, 300 pA and (b) +0.02 V, 280 pA. (c) Zoomed-in STM image of the area marked by the purple dashed rectangle showing the Kekulé-O distorted graphene structure (+0.05 V, 400 pA). (d) FFT image extracted from Fig. 1b. (e) Setpoint-current-dependent dI/dV spectra recorded at the "cross" position (+0.4 V), exhibiting a gap opening of 90 meV in graphene. (T = 4.5 K)