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Single Atom Catalyst at Work: Real-Time Imaging of Adatom-Promoted Graphene Growth on Nickel

Single adatoms are expected to be involved in several surface processes, including the growth of epitaxial graphene. We demonstrate, both experimentally and theoretically, the catalytic role of single metal adatoms during the synthesis at technologically relevant temperatures (≈700 K) of graphene flakes on Ni(111) [1], mostly characterized by an epitaxial top/hollow-fcc registry with the substrate [2]. Single Ni atoms, diffusing on the metal surface, are temporarily trapped at kink sites along the graphene flake edges and facilitate the incorporation of new C atoms in the graphene network. Scanning tunneling microscopy (STM) imaging at the millisecond time scale allowed us to identify the edge structure [3] and individual Ni adatoms, directly capturing their catalytic action. Force-field molecular dynamics (MD) and ab-initio density functional theory (DFT) calculations rationalize the experimental observations, giving a complete description of the growth pathways. Our results unveil the mechanism ruling the activity of a single atom catalyst at work [4].

References

[1] L. L. Patera et al., ACS Nano 7 (2013) 7901
[2] F. Bianchini et al., J. Phys. Chem. Lett. 5 (2014) 467
[3] L. L. Patera et al., Nano Lett. 15 (2015) 56
[4] L. L. Patera et al., Science. (2018) 359(6381):1243-1246.

Figures

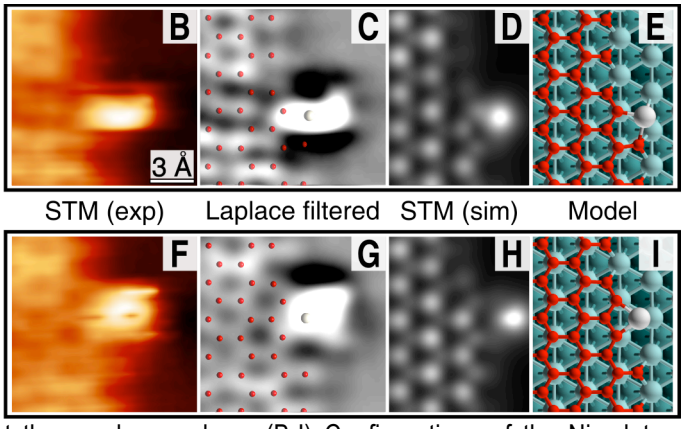

Figure 1: Nickel adatoms at the graphene edges: (B-I) Configurations of the Ni adatom at klein edge kinks: (B, F) Highspeed STM images, (C, G) Laplace-filtered images with superimposed ball models, (D, H) DFT simulation of constant height STM images based on the calculated geometries in (E, I).