Atomic Scale Insights into Layered 2D Materials Epitaxy, Dopants and Defects

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Layered 2D Materials in the monolayer limit are primarily surfaces and interface with other materials through van der Waals interactions. However, the presence of defects creates dangling bonds that act as binding sites and disrupt the periodic van der Waals bonding. Understanding the interfacial coupling between different 2D monolayers and with other atoms, molecules and materials at the atomic scale is essential for building accurate models, and transmission electron microscopy is a leading approach for studying atomic scale behavior. Here, aberration corrected scanning transmission electron microscopy, combined with electron energy loss spectroscopy is used to extract accurate insights into atoms and their local bonding in 2D materials and how epitaxy arises at the interfaces. This will include graphene, hBN and transition metal dichalcogenides of mixed form, including MoS2, WS2, SnS2, PtSe2, PdSe2 and more. Insights into the epitaxy in twisted Moire systems of 2D will be shown, and how 4D-STEM, figure 1, can be used to see structural insights beyond conventional imaging such as electric field mapping around single dislocations [1], figure 2. The atomic structure of several dopant atoms at the interface and the role of surface carbon adsorbates on the adatom adsorption and migration will be presented. These results will provide detailed information about how individual atoms behave on 2D surfaces that are suspended and under in-situ heating up to 1000^{o}C.

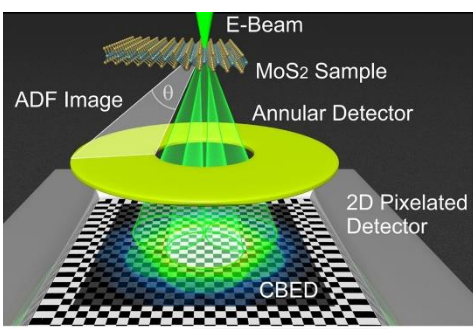

Figure 1 4D-STEM schematic

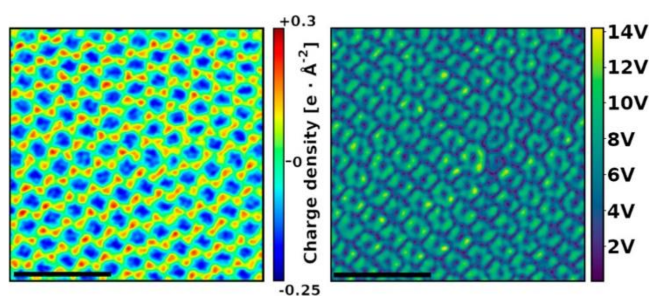

Figure 2 Total charge image (left) and electric field map (right) of dislocation core in graphene obtained from 4D-STEM

[1] M. Coupin, Y. Wen, S. Lee, A. Saxena, C. Ophus, C. Allen, A. Kirkland, N. Aluru, G-D. Lee, J. H. Warner, *Mapping Nanoscale Electrostatic Field Fluctuations Around Graphene Dislocation Cores Using 4D-STEM*, **Nano Letters**, 23, 6807-6814, (2023)

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