Atomic resolution electron microscopy and spectroscopy of ion implanted dopants in two-dimensional materials

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Research interest into single and few-layer transition metal dichalcogenides (TMDs) has increased rapidly in the past decade due to the reliable and reproducible methods of synthesis and sample preparation. Arguably the most studied TMD is MoS_2, a direct bandgap semiconductor in its single-layer form, transitioning to an indirect bandgap in its few-layer form [1]. MoS_2, along with other TMDs, has a host of interesting optoelectronic [2,3], physical [4] and spintronic [5] properties, possibly leading to various nanoscale devices which could outperform current designs. However, to create these nanoscale devices for real-life applications, we must understand the interaction they have with dopants and other materials.

Ion implantation is a vital tool used in semiconductor industry today, and for two-dimensional materials the technique provides a clean, controlled doping method [6]. For the first time, we have utilised ultra-low ion implantation (10-25 eV) to introduce substitutional Se dopants into monolayer MoS_2 [7]. Additionally, we have discovered the formation of Au nanoparticles (NP) on the surface of both MoS_2 and $MoSe_2$ after 10 eV Au ion implantation. Au NPs have been reported as p-type surface charge dopants in MoS_2 [8]. We have also carried out implantation with Mn and other transition metals to further develop the electronic properties of TMDs experimentally. Additionally, this method could be combined with ion beam masking to produce highly accurate and reproducible 2D material surface electrodes for contacting.

To investigate these substitutional and surface dopants we have employed high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM), electron energy loss spectroscopy (EELS) and energy dispersive x-ray spectroscopy (EDX). Aberration corrected STEM imaging, supported by image simulation, allow us to probe the local structure (dopant site, vacancies, defects) of our doped material, and movement of host atoms and substitutional ions. EELS, supported by density functional theory (DFT) calculations, reveal electronic and optical information at high spatial resolution, providing local band structure, plasmon and exciton information.

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