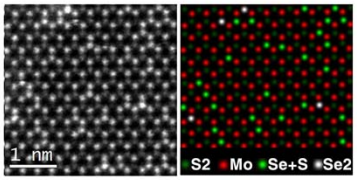
New imaging-based chemical analysis of atomic layers



Quantitative *Z*-contrast image analysis can translate an experimental image (left) of Se-doped MoS_2 into a map showing the distribution of each type of atom (right) with single-atom sensitivity and single atomic-layer discrimination. Based on the atomic concentrations, the local band gap can be determined.

Work was performed as a User Project at Center for Nanophase Materials Sciences, Rice Univ., Vanderbilt Univ., Pennsylvania State Univ., Shinshu Univ., Nanyang Technological Univ.

Scientific Achievement

Dopant atoms in two-dimensional materials have been located and quantified using a new *Z*-contrast image analysis method, which facilitates the ability to control dopant distribution to modify physical and chemical properties of materials.

Significance and Impact

Controlling and quantifying dopant concentration within each atomic layer of 2D ternary compounds provides an efficient method to modify their local electronic and chemical properties, and is of particular importance for practical applications of 2D materials.

Research Details

- Direct mapping of dopant distribution with single atom sensitivity and single-layer discrimination; measurement of local bandgap with resolution at the 10 nm level.
- Controlled synthesis of Se-doped MoS_2 with a wide range of doping levels.

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Dopant atoms in two-dimensional materials have been located and quantified using a new Z-contrast image analysis method. With this ability, the distribution of dopants can be verified as the physical and chemical properties are modified. As a demonstration of this control, the optical band gap of molybdenum disulfide has been tuned between 1.85 and 1.60 eV by changing Se concentration. Controlling and quantifying dopant concentration within each atomic layer of 2D ternary compounds provides an efficient method to modify their local properties, and is thus of particular importance for practical applications of 2D materials. The new quantitative Z-contrast image analysis method reported in our work[1] overcomes the main challenge of quantifying and locating the dopant atoms within each atomic layer, and achieves layer-by-layer mapping of dopants in a bilayer structure for the first time. Our results provide new insights into the growth mechanism and alloying behavior in 2D dichalcogenide atomic layers, and demonstrate that growth of uniform ternary 2D dichalcogenide alloy films with tunable electronic properties is feasible.

Reference:
"Band Gap Engineering and Layer-by-Layer Mapping of Selenium-Doped Molybdenum Disulfide"
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