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Adsorbates indicate if an insulator is Mott or not

A new experimental technique indicates the origins of a material's electronic behavior: from band structure or from electron–electron correlations.

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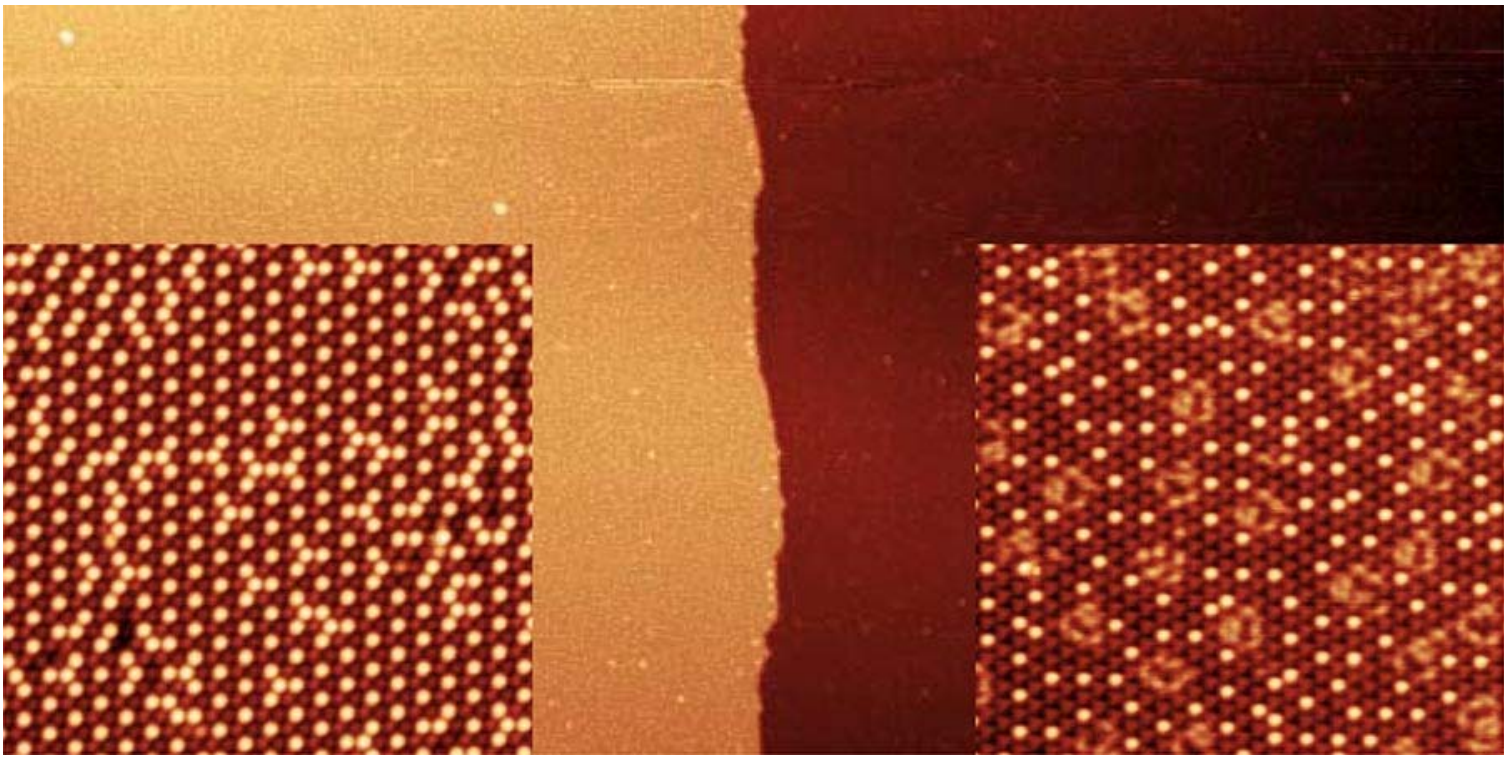
Conventional insulators have a large energy gap between the filled and unfilled electron states. Mott insulators have a half-filled electron band, and thus they would be metallic but for strong Coulomb interactions between the electrons that prevent electron flow.

Both conventional and Mott insulators yield identical electrical behavior. Determining whether a crystal is one or the other typically requires theory. The

trouble is, predictions can be contradictory and complicated, especially when charge-density waves and other insulating states are present. Now Han Woong Yeom of Pohang University of Science and Technology in South Korea and his colleagues have developed a direct experimental method that uses potassium atoms to help distinguish Mott and conventional insulators.

For their putative Mott insulator, the researchers picked layered tantalum disulfide, which has a charge-density-wave state. Although most models predict that trigonal (1T) TaS_2 is a Mott insulator, they do not account for electrons that can hop between layers. More recent models suggest that layers will pair up, share electrons, and become conventional insulators.

Yeom and his colleagues prepared a 1T-TaS_2 sample with two regions that differed in thickness by one layer. If the layers pair off, as other recent experimental results support, then one region would have a paired layer on top and the other would have a lone unpaired layer on top. In the absence of pairing, the two regions would behave the same.



A 400-by-200 nm scanning tunneling microscopy image of the two 1T-TaS_2 regions is overlaid with zoomed-in 30-by-30 nm images (left and right bottom corners). The bright dots indicate potassium atoms at the center of the charge-density-wave unit cells; on the right, the medium contrast blurs indicate K atoms between the center of neighboring unit cells. Credit: J. Lee, K.-H. Jin, H. W. Yeom, *Phys. Rev. Lett.* **126**, 196405 (2021)

The researchers deposited K atoms onto the exfoliated flake and then took scanning tunneling microscopy images to pinpoint their locations. The atoms distributed differently in the two regions, as seen in the images: At left, they ended up only at the center of the charge-density-wave unit cells; at right, the atoms also landed on an additional spot between the center of neighboring unit cells.

The real power of the K adsorbates became evident in the spectroscopic measurements. In the absence of adatoms, the two regions have insulating spectra with a bandgap of 250 meV in one region and 400 meV in the other. In the presence of adatoms, the TaS_2 layer gains an electron from each K atom. If the flake is a Mott insulator, the extra electron fills the electron orbital and its gap goes away, as observed in the region that has an unpaired top layer. If the flake is a conventional insulator, the extra electron shifts the energies but its gap remains, as observed in the regions with a paired top layer.

Without depending on theory, Yeom and his colleagues showed that a monolayer of 1T-TaS_2 is a Mott insulator. Their new experimental technique should help identify correlated states in a broad range of materials. (J. Lee, K.-H. Jin, H. W. Yeom, *Phys. Rev. Lett.* **126**, 196405, 2021.)

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