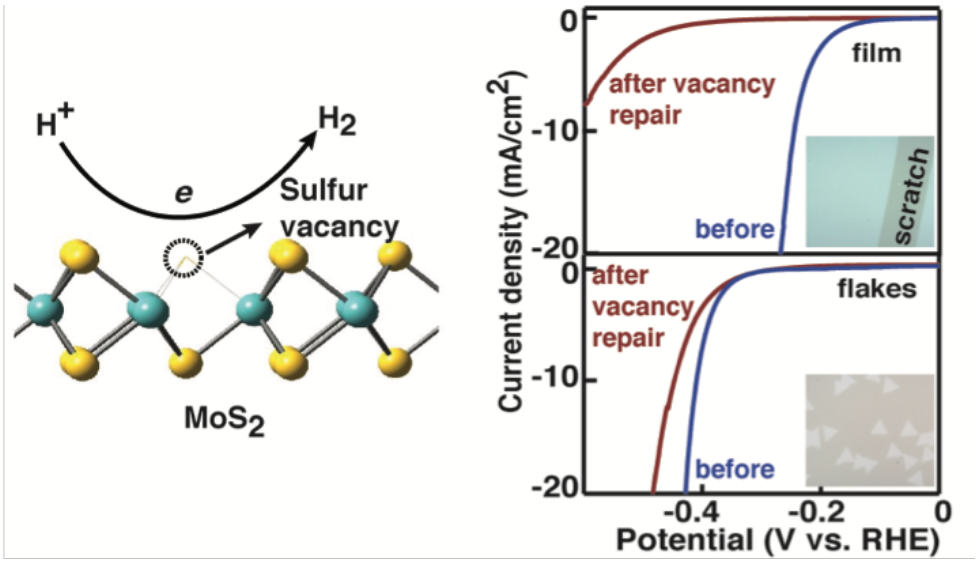
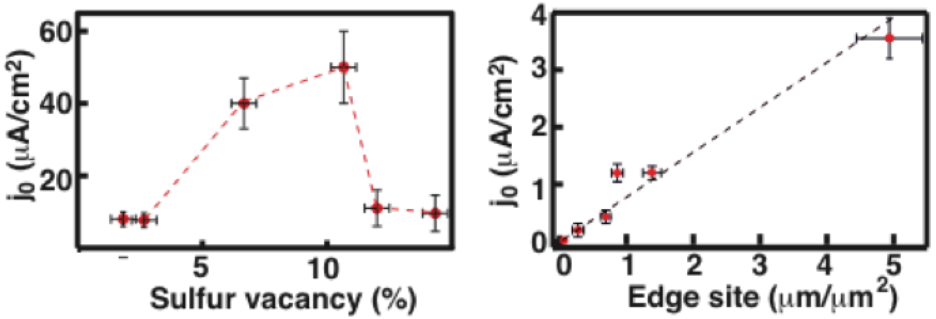
All The Catalytic Active Sites of MoS_2 for Hydrogen Evolution





Up left: schematic illustration for catalytic activity at sulfur vacancies in MoS2 for hydrogen evolution. **Up right**: Polarization curves of MoS2 monolayer films and monolayer flakes before and after being treated by the vacancy repairing process. Exchange current density as a function of the density of (**Bottom left**) sulfur vacancies and (**Bottom right)** edge sites;

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Work performed at NC State, Duke, and Brookhaven National Lab

Scientific Achievement

1. For the first time quantitatively evaluate the catalytic activities of all possible sites at MoS2, edge sites, sulfur vacancies, and grain boundaries.
2. Unambiguously demonstrate that the sulfur vacancies of MoS_2 may have strong catalytic activities for hydrogen evolution while grain boundaries only show weak activity. This defies the common sense, which believes only edge sites are catalytic active.

Significance and Impact

The result points out the best strategy to enable MoS2 materials as high-performance cost-effective catalyst for hydrogen evolution is engineering sulfur vacancies, in stead of engineering the edge sites that has been extensively used by the community.

Research Details

We have examined the catalytic activity of MoS2 as a function of physical features controlled in atomic-scale precision by synergistic efforts in theoretical and experimental ground.

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