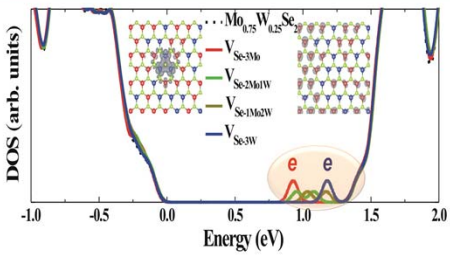
Alloy Engineering Cleans Up a New Class of Semiconductors



The electronic density of states of defective $Mo_{1-x}W_xSe$ alloys, demonstrating the suppression of deep defect levels. **Left inset**: the charge densities of the in-gap *e* levels of V_{Se} in $Mo_{0.75}W_{0.25}Se_2$ (V_{Se-3W}). **Right inset**: the charge densities of the conduction band minimum for $Mo_{0.75}W_{0.25}Se_2$.

Work was performed at the Center for Nanophase Materials Sciences, University of Utah and NREL.

Scientific Achievement

Simulations provide a recipe based on mixing of two materials ("alloying") to remove defect levels that limit the optimal electronic and optoelectronic properties of semiconductors.

Significance and Impact

By reducing undesired energy levels for electrons (in-gap deep levels) while maintaining the key electronic properties, the carrier density can be improved by 5 orders of magnitude (i.e., 100,000 times).

Research Details

- First-principles calculations demonstrate the novel concept of deep defect level suppression in 2D transition metal dichalcogenide alloys.
- Calculations for $Mo_{1-x}W_xSe_2$ were based on quasirandom structures with different W concentrations to identify feasible defect structures.

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Narrative Highlight Text: Specific alloying is shown to provide an effective means to suppress the deep defect levels in semiconductors while maintaining their basic electronic properties. Specifically, for transition-metal dichalcogenides, such as $MoSe_2$ and WSe_2, where anion vacancies are the most abundant defects that can induce deep levels, the deep levels can be effectively suppressed in $Mo_{1-x}W_xSe_2$ alloys at low W concentrations. This surprising phenomenon is associated with the fact that the band edge energies can be substantially tuned by the global alloy concentration, whereas the defect level is controlled locally by the preferred locations of Se vacancies around W atoms. These new findings illustrate a concept of alloy engineering and provide a promising approach to control the defect properties of
Semiconductors where applications in electric and optoelectronic devices depends critically on controlling their band structures and defect properties.

Reference:

"Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in Transition-Metal Dichalcogenides"
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