

"Predicting the Gas Sensing Performance of 2D Materials"

Special Seminar

Tuesday, August 2, 2022
1:30 - 2:30 p.m. BRWN 4102

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Abstract:

We study the potential of material simulations based on first-principles methods to predict gas sensing properties of 2D materials. This emerging class of materials is of particular interest to gas sensing applications due to high surface-to-volume ratios and chemical stability. We discuss in detail results of electron transport calculations within the Landauer-Büttiker formalism and compare the conclusions to analyses in terms of adsorption energies, charge transfers, and work functions. Specific examples include the effects of the interlayer interaction in bilayer MoS₂ and WS₂ on the gas sensing performance and the consequence of the presence of reactive Si in Si₂BN. We also address the properties of C₃N and para/meta-C₃Si. Potential of very sensitive gas sensing is demonstrated for para-C₃Si and is explained by the susceptibility of Dirac states to symmetry breaking distortions rather than by a mechanism based on charge transfer. Finally, the enhanced gas sensing performance of monovacant C₆BN is studied and it is shown that the work function changes of both pristine and monovacant C₆BN during gas adsorption do not correlate with the changes observed in the I-V characteristics.