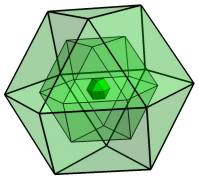
Materials Science Seminar
20/09/2022 11:30
Paoluzi room



Predicting the Gas Sensing Performance of 2D Materials

UDO SCHWINGENSCHLÖGL
Physical Science and Engineering, KAUST

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 MoS_2 and WS_2 on the gas sensing performance and the consequence of the presence of reactive Si in Si_2BN. We also address the properties of C_3N and para/meta-C_3Si. Potential of very sensitive gas sensing is demonstrated for para-C_3Si 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 C_6BN is studied and it is shown that the work function changes of both pristine and monovacant C_6BN during gas adsorption do not correlate with the changes observed in the I-V characteristics.