Improved Charge Transfer and Barrier Lowering across a Au–MoS2 Interface through Insertion of a Layered Ca2N Electride

Fouad Kaadou, Jesse Maassen and Erin R. Johnson

Department of Physics and Atmospheric Sciences, Dalhousie University, NS, Email: fouad.kaadou@dal.ca

Transition-metal dichalcogenides (TMDCs) are a family of layered semiconductors that offer great potential in the upcoming field of two-dimensional (2D) electronics. In particular, MoS2 is a TMDC with a desirable band gap for the construction of transistors, solar cells, and biochemical sensors. However, MoS2 layers lack any dangling out-of-plane bonds, making it challenging to form the proper electrical contacts required in any practical device. In this talk, I will discuss how the insertion of a 2D layered electride like Ca2N, an electron-rich material, at a metal-MoS2 interface may remedy this problem. As a proof-of-concept, we study a Au-Ca2N-MoS2 heterostructure within a density-functional theory (DFT) framework using the exchange-hole dipole moment (XDM) dispersion model. We choose Au since it is a common contact metal, its interface with MoS2 is well characterised, and it exhibits strong Fermi-level pinning, as well as high Schottky and tunneling barriers. The insertion of Ca2N eliminates both the tunneling and Schottky barriers through nearly complete charge transfer from the electride surface states. The resulting Au-Ca2N-MoS2 heterostructure shows features of a true ohmic contact. Our promising results may indicate that the insertion of an electride may solve the more general metal-TMDC contact problem.