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Electronic and Chemical Structure of 2D materials

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The drive to produce smaller, faster, lower power electronic components for computing is pushing the semiconductor industry to nanometer-scale device structures. Atomically thin two-dimensional (2D) materials such as transitional metal dichalcogenides (TMDs) and graphene are a promising class of materials for nanoelectronics with unique optical and electronic properties. The properties of mono- to few-layer TMDs are highly sensitive and reactive to their local environment (ambient conditions and adsorbates) and the interfaces within a fabricated device structure (gate dielectric, contacts), which can all impact their electronic properties and extrinsic device characteristics. Here, we will present the electronic and chemical structure of doped graphene on silicon carbide and polymorphs of molybdenum telluride.

Large area epitaxial graphene (EG) grown on silicon carbide (SiC) provides a feasible route to scalable production of graphene-containing electronic components. EG on SiC display strong n-type (electron) doping due to the interaction of the zero-layer graphene [1] that is directly bonded to SiC. Nitric acid has been shown to be an effective p-doping agent and produce low carrier density of EG [2]. Using laboratory-based ultraviolet (UPS) and x-ray photoelectron (XPS) spectroscopies, we investigate the surface chemical composition and electronic structure of nitric acid exposed EG on SiC. We observe the presence of nitrogen on the surface which provides direct evidence on the role of nitric acid as extrinsic dopant of EG on SiC. The UPS results indicate that the EG surface is that of a semi-metal after exposure to nitric acid. Technological commercialization of graphene for electronic components requires that their electronic properties be engineered for specific device functionality such as the charge carrier density.

With the vast elemental phase space of TMDs, TMDs have a range of electronic properties giving rise to metallic, semiconducting, or insulating properties. In addition, some TMDs exhibit polymorphism and different packing geometry or phase can distinctly impact the electronic structure and it will influence optical and transport properties. Molybdenum telluride ($MoTe_2$) can exist in three phases: 2H, 1T, and 1T'. The 2H phase is semiconducting, while the other phases are metallic or semi-metallic. For the bulk 2H $MoTe_2$ crystal, the surface is relatively stable and with little oxidation based on our XPS and UPS results. This is not the case for the 1T' phase of crystalline $MoTe_2$, where the molybdenum and tellurium atoms at the surface are significantly oxidized. The 1T' phase can be cleaved at the surface, and we can observe the semi-metallic properties by angle-resolved photoemission. The cleaved 2H $MoTe_2$ surface exhibits dispersion of the valence bands and a valence band maximum consistent with being an n-type semiconductor. $MoTe_2$ is appealing for manufacturing of nanoelectronic components due to tunability in electronic properties in one material system. Continued innovation requires novel nanoelectronic materials and devices, coupled with a thorough understanding of the electronic structure which determines device functionality.

[1] P. Mallet, F. Varchon, C. Naud, L. Magaud, C. Berger, and J.-Y. Veuillen, Phys. Rev. B 76, 041403 (2007).

[2] Y. Yan, L.-I. Huang, Y. Fukuyama, F.-H. Liu, M. A. Real, P. Barbara, C. -T. Liang, D. B. Newell, and R. E. Elmquist, Small 11, 90 – 95 (2015).