Molecular Sensing at Graphene Grain Boundaries

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Abstract:

In this study, we introduce the graphene GBs as an ideal structure for detection of toxic analytes. To this objective, we fabricated individual graphene GB based sensor and study their gas sensing characteristics by exposing against the dimethyl methylphosphonate (DMMP) or 1,2-dichlorobenzene (DCB) gas molecules. DMMP is an electron donor while DCB is electron acceptor molecules. We uncovered that an isolated graphene GB has ~300 times higher sensitivity to gas molecules than a single crystalline graphene grain. We also investigated the sensing response of a sequence of multiple GBs, naturally formed by the merging of the grains in the CVD growth. Our results show a clear sensing cross-over from a single GB toward a polycrystalline sensor, as the number of GBs are increased from 1 to more than 5. Our hybrid modeling of an electronic structure and transport in realistic GBs reveals that the ultra-sensitivity in GBs is caused by a synergetic combination of gas molecules accumulation at GB, together with the existence of ultrasensitive switchable transport channels in GBs. The discovered sensing platform opens up new pathways for the design of nanometer scale highly sensitive chemical detectors.

Keywords: Grain boundary, Graphene, Sensors, Transmission spectrum