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**Gas sensing of a saturated tin/defective graphene device** SHERIF TAWFIK, School of Physics, The University of Sydney, Sydney, 2006 NSW, Australia, X. CUI, Australian Key Centre for Microscopy & Microanalysis, The University of Sydney, Madsen Building F09, NSW 2006, Australia, DAMIEN CARTER, Nanochemistry Research Institute, Curtin University, GPO Box U1987, Perth, WA 6845, Australia, S. RINGER, Australian Key Centre for Microscopy & Microanalysis, The University of Sydney, Madsen Building F09, NSW 2006, Australia, C. STAMPFL, School of Physics, The University of Sydney, Sydney, 2006 NSW, Australia — The sensitivity and selectivity of defective graphene to gases is enhanced by implanting single metal adatoms into vacancy sites. Knowledge of the behavior of these devices under the incremental adsorption of gas molecules until saturation is essential for determining the sensitivity of the device in realistic situations as well as for evaluating the applicability of the device in molecular capture and storage. We present a DFT study of incremental gas adsorption of $CO_2$, $NO_2$, $SO_2$ and $H_2S$ gases on tin adatom-double vacancy graphene system, in the presence and absence of $O_2$. Within the NEGF formalism, we analyze the sensitivity and selectivity of the saturated device to the gas species, showing distinctive transport features for each of the gas species.

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