Simulation Study of Electrical and Optical Properties of 2D-Material FETs

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Two-dimensional (2D) semiconductor materials can provide unique and favorable physical properties for the next-generation electronic and optoelectronic device applications. Among transition metal dichalcogenides (TMDCs), molybdenum disulfide (MoS_2) has been most extensively explored for field-effect transistor (FET) switching and photonic devices due to its high field-effect mobility (μ_{eff} ~700 cm^2/V-s) and high photoresponsivity (R ~900 A/W).[1–8] Quite recently, a new 2D material of layered black phosphorus (BP or phosphorene) was also investigated for switching devices.[9–11]

Using self-consistent atomistic quantum transport simulation based on non-equilibrium Green's function (NEGF) formalism, we investigate various 2D materials such as black phosphorus and TMDCs for FET applications. We discuss comprehensive device characteristics including short-channel effects, subthreshold swing, I_{on} vs. I_{on}/I_{off}, and the effects of multiple layers for both high-performance and low-power applications. We also show our simulation results for optoelectronic applications where photoconductive (PC) and photovoltaic (PV) effects in 2D materials are discussed in detail. In particular, modeling/simulation of photocurrent is described, and strategies for higher responsivity in 2D material based phototransistors are introduced.

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