Abstract Submitted
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First-principles Simulations of a Graphene-Based Field Effect Transistor[1] YUN-PENG WANG, HAI-PING CHENG, Univ of Florida - Gainesville — We propose a first-principles method to simulate the effect of a gate voltage on a two-dimensional channel. Because of the aperiodic structure of field effect devices, we adopt the effective screening medium (ESM) method, which enables us to solve the Poisson equation with free boundary conditions, to simulate nanoscale field effect devices. With this approach, we investigated a graphene-based vertical field effect tunneling transistor with a graphene|h-BN|graphene multilayer structure. The calculated carrier density on the graphene away from the gate electrode is sublinear with respect to the gate voltage, and decreases as the thickness of the h-BN barrier increases. The band structure of graphene layers near the Fermi energy exhibit a $\sim 0.05\,\mathrm{eV}$ gap opening due to interactions with h-BN, as well as the chemical potential difference between the two graphene monolayers. This work paves the road to first-principles simulations of nanoscale field effect transistors and opens a new avenue towards computational guided device design.

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Yun-Peng Wang
Univ of Florida - Gainesville

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