Efficiency of Gate Control in Short-Channel Pt-WSe_2-Pt Nanojunctions: A First-Principles Study

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Abstract

Enhancing the electrical connectivity between metal leads and monolayer transition metal dichalcogenides poses a critical challenge in the advancement of next-generation field-effect transistors. Our study sought to integrate h-AlN as an insertion layer in the Pt-WSe_2-Pt field-effect transistor, aiming to diminish contact resistance and evaluate the influence of current density. The non-equilibrium Green's function, in conjunction with density functional theory, was employed to compute the transmission coefficient under both equilibrium and non-equilibrium conditions. The findings suggest that incorporating a single layer of h-AlN may not lead to significant improvements in current density, as the Pt-WSe_2-Pt with h-AlN exhibits a diminished p-type character. Meanwhile, a scaling factor for gate-controlling efficiency was introduced to reconcile the current calculations under non-equilibrium conditions with the Landauer formula incorporating the equilibrium transmission function. Nevertheless, a non-linear effect may need to consider for the scaling factor for gate-controlling efficiency. We recommend that the approach outlined in this study be replicated in other theoretical plants.

Keywords - FET, TMD, NEGF, Landau formula.