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Development of an ab-initio calculation method for 2D layered materials-based optoelectronic devices HAN SEUL KIM, YONG-HOON KIM, Korea Advanced Institute of Science and Technology — We report on the development of a novel first-principles method for the calculation of non-equilibrium nanoscale device operation process. Based on region-dependent Δ self-consistent field method beyond the standard density functional theory (DFT), we will introduce a novel method to describe non-equilibrium situations such as external bias and simultaneous optical excitations. In particular, we will discuss the limitation of conventional method and advantage of our scheme in describing 2D layered materials-based devices operations. Then, we investigate atomistic mechanism of optoelectronic effects from 2D layered materials-based devices and suggest the optimal material and architecture for such devices.

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