Quantum simulation of semiconductor-based materials for THz and power device applications

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Two cases of quantum simulation of semiconductors will be presented. One is the structural, electronic/magnetic origin and mechanism of two-step photon absorption (TSPA) of low-temperature GaAs (LT-GaAs) obtained from density functional theory calculations and projected-augmented wave method. TSPA has been proposed to drive the below band-gap adsorption making possible the LT-GaAs-based photoconductive antenna pumped at 1560nm to exhibit bandwidths of ~4.5 THz. Another is the theoretical confirmation of XPS study of GaN used in high-electron-mobility transistors (HEMTs), showing the presence of Ga_2O sub-oxide (note solely Ga_2O_3 as generally accepted), will be discussed. The theoretical confirmation is derived from Ga-3*d* core-level shift calculations, among others.