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Development of a density functional theory approach for calculating electronic band structure parameters in support of Monte Carlo simulations of photoemission

Tuesday 3 June 2025 16:00 (2 hours)

Monte Carlo simulations are a powerful tool for modeling photoemission from photocathodes, enabling the prediction of key parameters such as quantum efficiency, mean transverse energy, electron spin polarization, and photocathode response time. However, these simulations require material band structure parameters, which are not always available from experiments. This work aims to establish a reliable framework for calculating electronic band structure parameters using Density Functional Theory (DFT). Specifically, we apply this framework to investigate the effects of lattice strain and temperature on the electronic band structure and electron transport in GaAs. This approach will be further extended to explore band structure modifications in heavily p-doped semiconductors and to calculate electronic band structures of novel spin-polarized photocathode materials.

Footnotes

Paper preparation format

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