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Investigating Ultra-Low Energy Ionization Yield from Nuclear Recoils in Semiconductor Detectors via Molecular Dynamics Simulations

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Nuclear recoil ionization yield constitutes a critical uncertainty source in low-energy detection for dark matter (DM) and coherent elastic neutrino-nucleus scattering (CEvNS) experiments. We present a novel methodology employing molecular dynamics simulations to assess ionization yields in crystalline semiconductor detectors. This non-parameterized approach resolving inherent limitations of traditional Lindhard model through explicit incorporation of crystal condensed matter effects, facilitating a seamless reliability from high-energy (>10 keV) to electron-hole pair (EHP) regimes. Our model achieves the best agreement with experimental data in silicon to date, especially at the minimal energy level of a single EHP. Meticulously consideration of ion transport mechanisms reveals fundamental ionization yield distributions, superseding conventional single-value models. The distributional paradigm extends the DM-nucleon elastic scattering exclusion limit to 0.29 GeV/c² under single-EHP sensitivity. We further report advancements in modeling quantum effects and channeling phenomena affecting ionization yields in high-purity germanium detectors.

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