Contribution ID: **121** Contribution code: **TUP030** Type: **Poster Presentation**

Development of a Density Functional Theory Approach for Calculating Electronic Band Structure Parameters in Support of Monte Carlo Simulations of Photoemission

Tuesday 12 August 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.

Please consider my poster for contributed oral presentation

No

Would you like to submit this poster in student poster session on Sunday (August 10th)

Yes

Footnotes

Funding Agency

I have read and accept the Privacy Policy Statement

Yes

Author: MENDEZ, Joniel (Northern Illinois University)

Co-authors: CALLAHAN, John (Northern Illinois University); CULTRERA, Luca (Brookhaven National Laboratory); CHUBENKO, Oksana (Northern Illinois University); Dr PALAI, Ratnakar (University of Puerto Rico at Río Piedras); KARKARE, Siddharth (Arizona State University)

Presenter: MENDEZ, Joniel (Northern Illinois University)

Session Classification: TUP: Tuesday Poster Session

Track Classification: MC1 - Colliders and other Particle and Nuclear Physics Accelerators