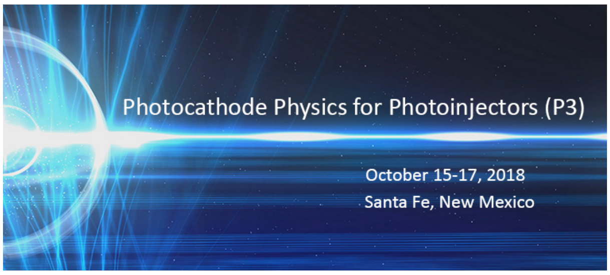


Contribution ID: **68** Type: **not specified**

# Predictive QE Models for PIC Codes Using DFT, TMA, Delay Models, and Optical Models

*Wednesday 17 October 2018 11:55 (20 minutes)*

High brightness photo-generated electron bunches for next generation and x-ray FEL's and light sources rely on particle-in-cell codes used for their modeling and design. The codes in turn require predictive and accurate models of photocathode yield, emittance, emission promptness and beam characteristics based on accurate material and environmental parameters, but in a but in a manner that does not computationally burden beam optics codes. In the present talk, three levels of theory and modeling are described ranging from existing models using simple and/or empirical input to models under development relying on advanced materials physics techniques.

1. Basic[1]: how a simple Fowler-DuBridge 1D photoemission model results from the same theory giving rise to thermal and field emission models and how a Moments-based distribution function approach gives yield and emittance using empirical optical and material parameters in a no-scattering approximation.
2. Modifications[2,3,4]: how transmission probabilities for triangular barriers are included; how scattering effects and delayed emission effects modify the emitted bunch and result in emission tails governed by the number of scattering events and the energy loss associated with them; and how a Lorentz-Drude model for metals allows optical constants such as reflectivity and penetration depth to be found for arbitrary wavelengths.
3. Augmentations[5,6]: How Density Functional Theory simulations are incorporated for the prediction of density of states, hyperbolic dispersion relations, and optical constants; how optical parameters from DFT results provide input to Lorentz-Drude (metal) and Adachi (semiconductor) models; how Airy function Transfer Matrix Approaches are used to treat resonant and reflectionless barrier and well structures and heterostructures; how Point Charge Models are used to describe surface roughness and shielding effects for random and periodic array surfaces.

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**Session Classification:** Session 10

**Track Classification:** Session 10: Theory and Computation - continued