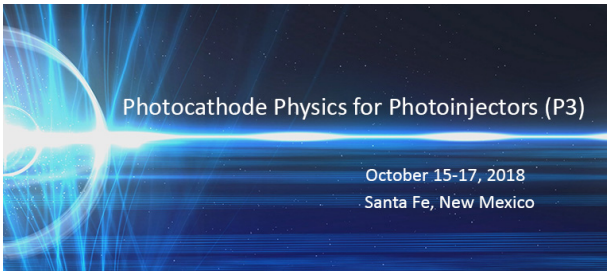

Contribution ID: **57** Type: **not specified**

Perspectives on Alkali Antimonide Semiconductors from Density-Functional Theory

Wednesday 17 October 2018 09:00 (20 minutes)

In calculating materials properties, a density-functional theory (DFT) has come to represent many functional theories, as well as many-body concepts that go beyond ground-state and density-dependent properties. The average practitioner should be aware of the complexion of DFT. We will outline the modern usage of DFT and its applicability to Alkali Antimonides; specifically, the density of states, index of refraction, reflectivity and other relevant parameters for photoemission models are calculated. As usual, no DFT works very well without interface with experimenters, so we summarize what we have learned about these materials from the existing literature and ask what needs to be determined through experiment.

Presenter: Dr FINKENSTADT, Dan (U.S. Naval Academy)

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