Contribution ID: **1409** Type: **Poster (Student, In Competition) / Affiche (Étudiant(e), inscrit à la compétition)**

Electron Localization in Group III-V Semiconductor Compound Alloys

Tuesday, 14 June 2016 19:14 (2 minutes)

We explore the band structures of new III-V material zinc blende alloys composed of B, N, Ga, As, In, Sb, and Bi for 1.55 μm wavelength telecommunication lasers and their corresponding electron localization at atomic sites from first principles. Engineering III-V semiconductors by mixing modifies their electronic properties including band gaps and lattice constants that are typically a blend of the original compounds and elements. Isoelectronic elements often result in undesirable effects. Electron localization in the vicinity of band edges affects the efficiency of carrier transport and recombination in lasers and solar cells. A new method has been developed to determine the electron localization from muffin tin radii (atomic sites) using the scheme of outlier detection with quartiles of electron probabilities. The advantage of this method is the ability to distinguish a strongly localized electron within the atomic muffin tin radius from a baseline of delocalized electrons. Comparing the results with the unfolded band structures'Bloch character; the outlier method is in general agreement. The industry standard of InGaAs for 1.55 μm is shown to have the least amount of localized electronic states near the band edges. Alternatively, we find that the electron localization is increased, noticeably with the addition of B and Bi, which affects both radiative and non-radiative recombination rates. To accommodate future Group III-V semiconductor band engineering, we suggest design criteria to facilitate the prediction of localization in new alloys.

Primary author: PASHARTIS, Christopher (McMaster)

Co-author: RUBEL, Oleg (McMaster University)

Presenter: PASHARTIS, Christopher (McMaster)

Session Classification: DCMMP Poster Session with beer / Session d'affiches, avec bière DPMCM

Track Classification: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)