



Contribution ID: 490

Type: Oral Presentation

## Accurate model of Si-Ge-Sn alloys: Electronic and Optical properties

*Thursday, 12 July 2012 14:30 (20 minutes)*

### Abstract content <br> &nbsp; (Max 300 words)

A method based on the tight-binding linear muffin-tin orbital (TB-LMTO) and the Quasiparticle Self-consistent GW (QSGW) approximation is discussed. The goal is to obtain accurate electronic and optical properties of semiconductor alloys.

In this new approach, the parameters of the TB-LMTO Hamiltonian are used to fit the difference in the QSGW self-energies and the LDA exchange-correlation potentials. As such, the method possesses the accuracy of the QSGW approximation and the efficiency of the TB-LMTO.

We use the new Hamiltonian to interpret the optical transitions in Si-Ge-Sn alloys.

### Apply to be<br> consider for a student <br> &nbsp; award (Yes / No)?

No

### Would you like to <br> submit a short paper <br> for the Conference <br> Proceedings (Yes / No)?

Yes

**Primary author:** Dr AZEMTSA DONFACK, Hermann (University of South Africa)

**Co-author:** Prof. VAN SCHILFGAARDE, Mark (King's College London)

**Presenter:** Dr AZEMTSA DONFACK, Hermann (University of South Africa)

**Session Classification:** DCMPPM2

**Track Classification:** Track A - Division for Condensed Matter Physics and Materials