

Abstract Submitted  
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**How does atomic microstructure of alloys affect electronic structure: The case of InGaN<sup>1</sup>** J.A. CHAN, NREL, J.Z. LIU, Monash University, A. ZUNGER, NREL — The atomic microstructure of alloys is rarely perfectly random, exhibiting instead differently shaped precipitates, clusters, zig-zag chains, etc. While its expected that such microstructural features will affect the electronic structure carrier localization, band gaps), theoretical studies have until now been restricted to investigate artificial “guessed” microstructural features. We have *derived* the equilibrium alloy microstructure of InGaN using (i) density functional total energies of  $\sim 50$  ordered structures to construct a (ii) multi-body cluster-expansion, including strain effects to which we have applied (iii) Monte Carlo simulations, giving the T-x phase diagram of bulk and epitaxial alloys as well as their atomic microstructure [1]. The ensuing electronic structure associated with the microstructure was then determined by applying empirical pseudopotentials. We catalogue the manner in which microstructure affects electronic structure and investigate how the hole localization and band level energies correlate with In concentration, strain and particular structural motifs formed in equilibrium. [1] J.Z. Liu, and A. Zunger, Phys. Rev. B, **77**, 205201 (2008), J.Z. Liu *et al*, Phys. Rev. Lett. **99**, 145501 (2007).

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Jennifer Chan  
NREL

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