The role of N-H complexes in the control of localized center recombination in hydrogenated GaInNAs

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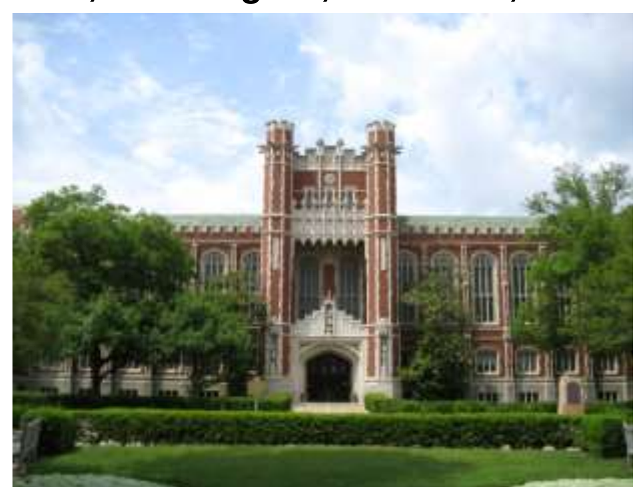
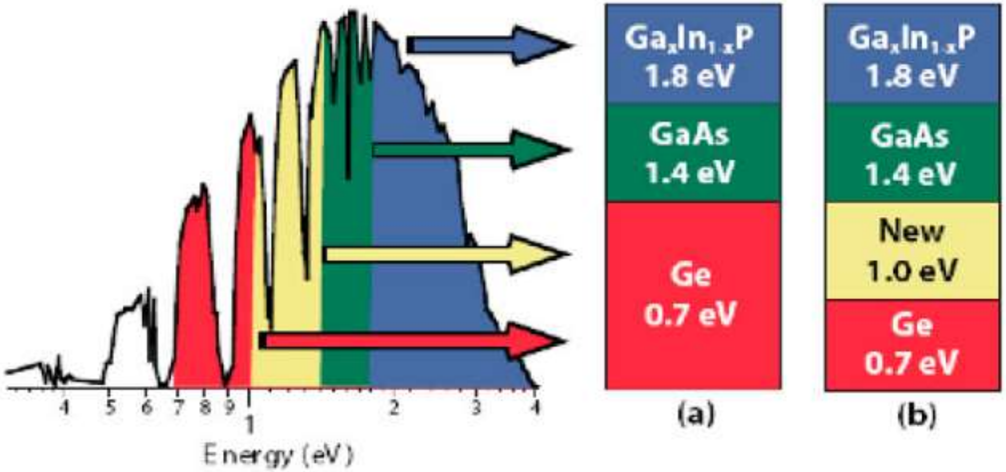
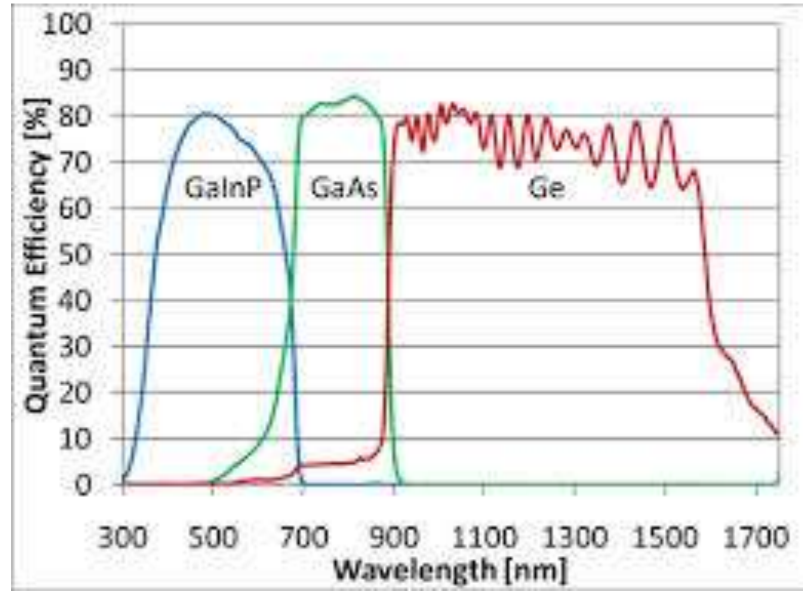


Multijunction Solar Cells: Divide and Conquer



J.F. Geisz and D.J.Freidman, Semiconductor Science and Technology 17, 769 (2002)

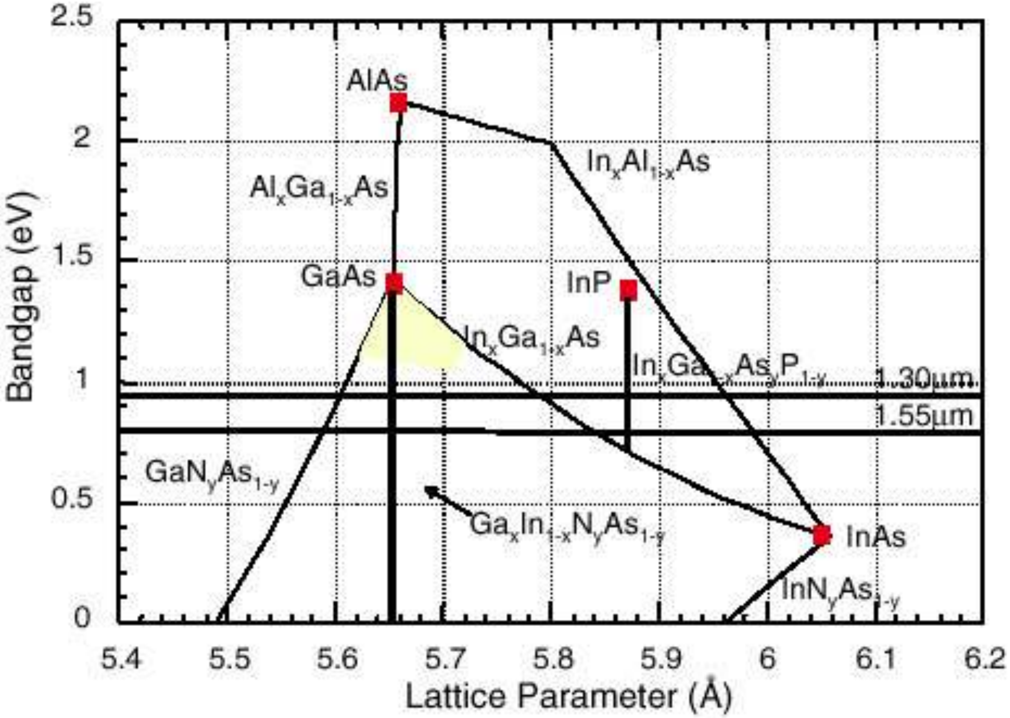


http://www.pvmeasurements.com/

- Three junctions: 44% efficient
- Four junctions: Up to 52% efficient
- Power wasted by Ge due to poor current matching

We need a material with 1eV band gap, correct lattice spacing

GaInNAs is a Promising but Problematic Candidate for the Fourth Junction



J. S. Harris, Semicond. Sci. Technol. 17, 880 (2002)

Growth Problems:

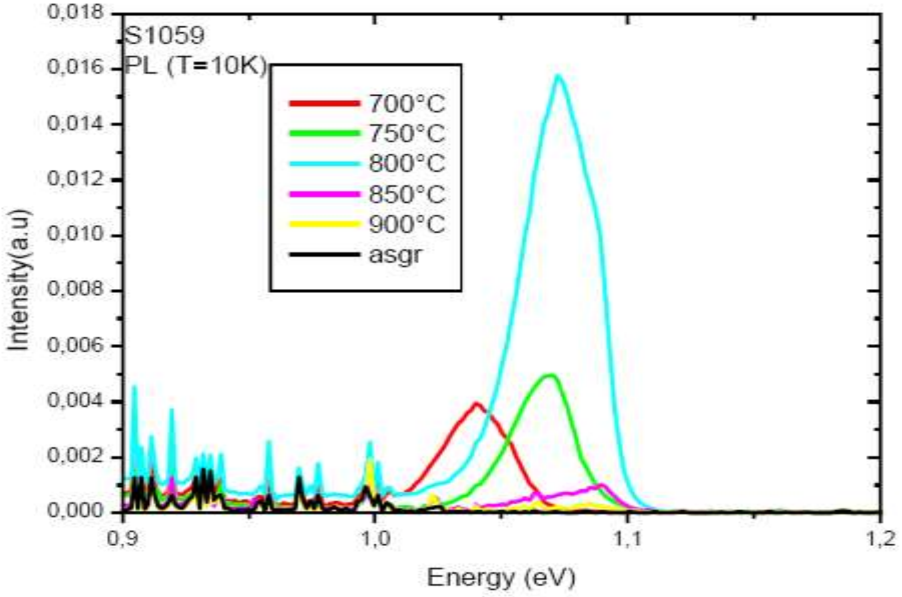
- High temperature--phase separation, clustering
- Low temperature--defect formation, low nitrogen inclusion

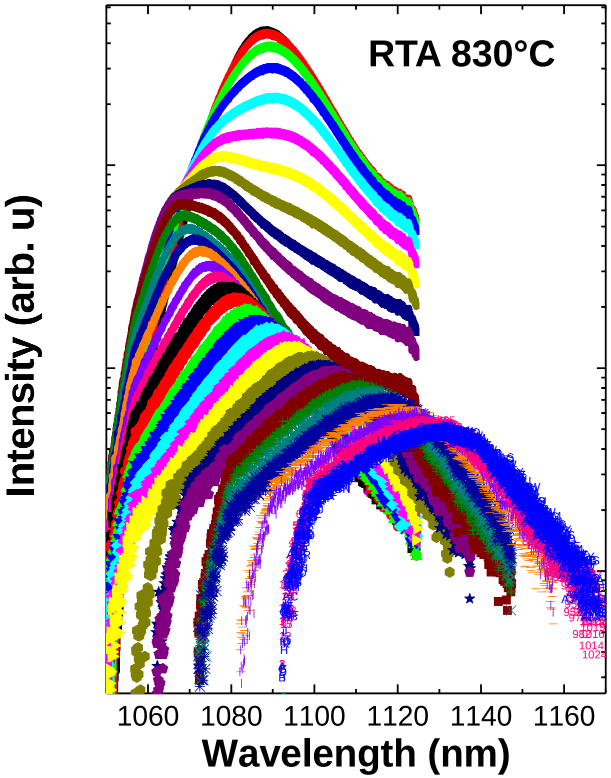
Regardless of sample quality, substitutional N is locally different electrically than As, causing low diffusion lengths.

Effects of Annealing

<u>Post – growth annealing improves material quality</u>

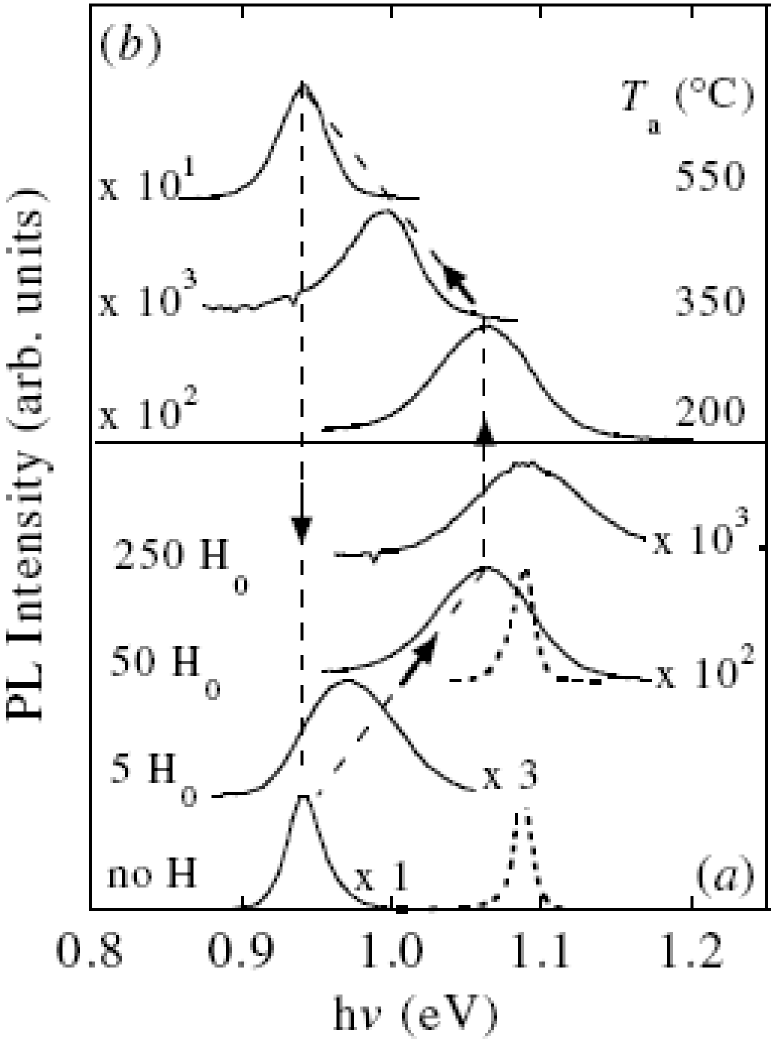
- Ga-vacancies removed
- N – As exchange increase nitrogen incorporation
- Low temperature PL dominated by localization centers





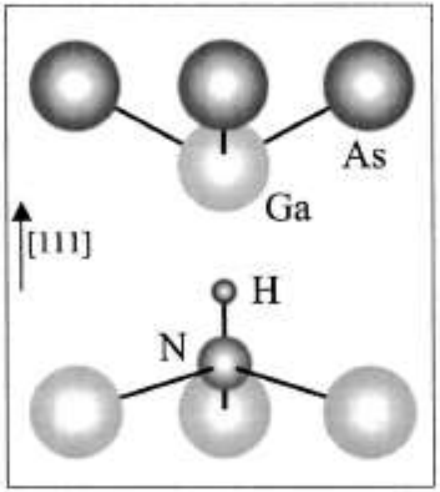
Effects observed in the performance of GaInNAs solar cells

Hydrogenation Has Shown Passivation of Substitutional Nitrogen



Polimeni *et al*. Semi. Sci Tech. **797,** (2002)

- Restoration of original band gap
- Process reversible through annealing
- Favorable due to small, electronegative nitrogen



Bissiri *et al*. Phys. Rev. B. **65**, 235210 (2002)

Selective Defects Passivation in Solar Cell Materials

Oklahoma Center for the Advancement of Science and Technology

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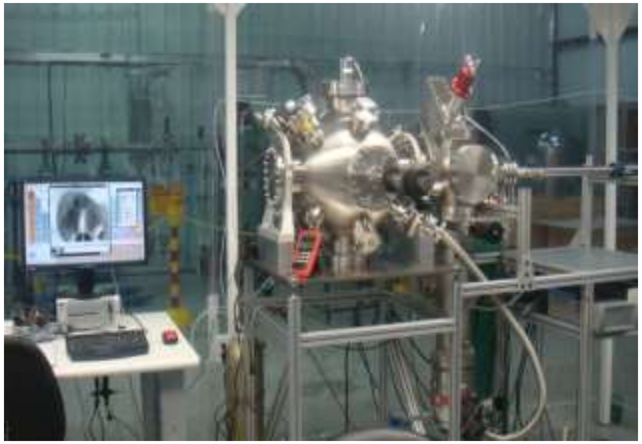
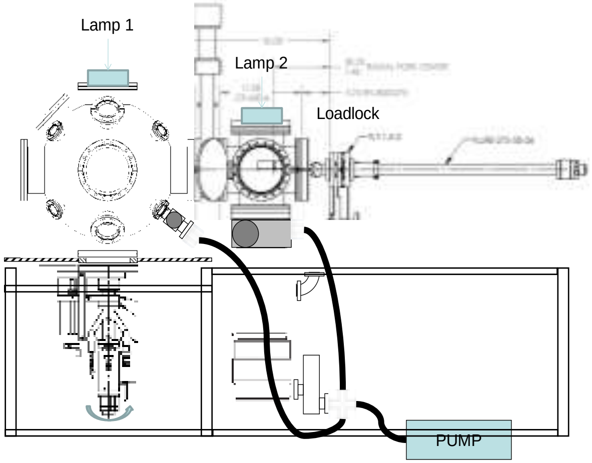
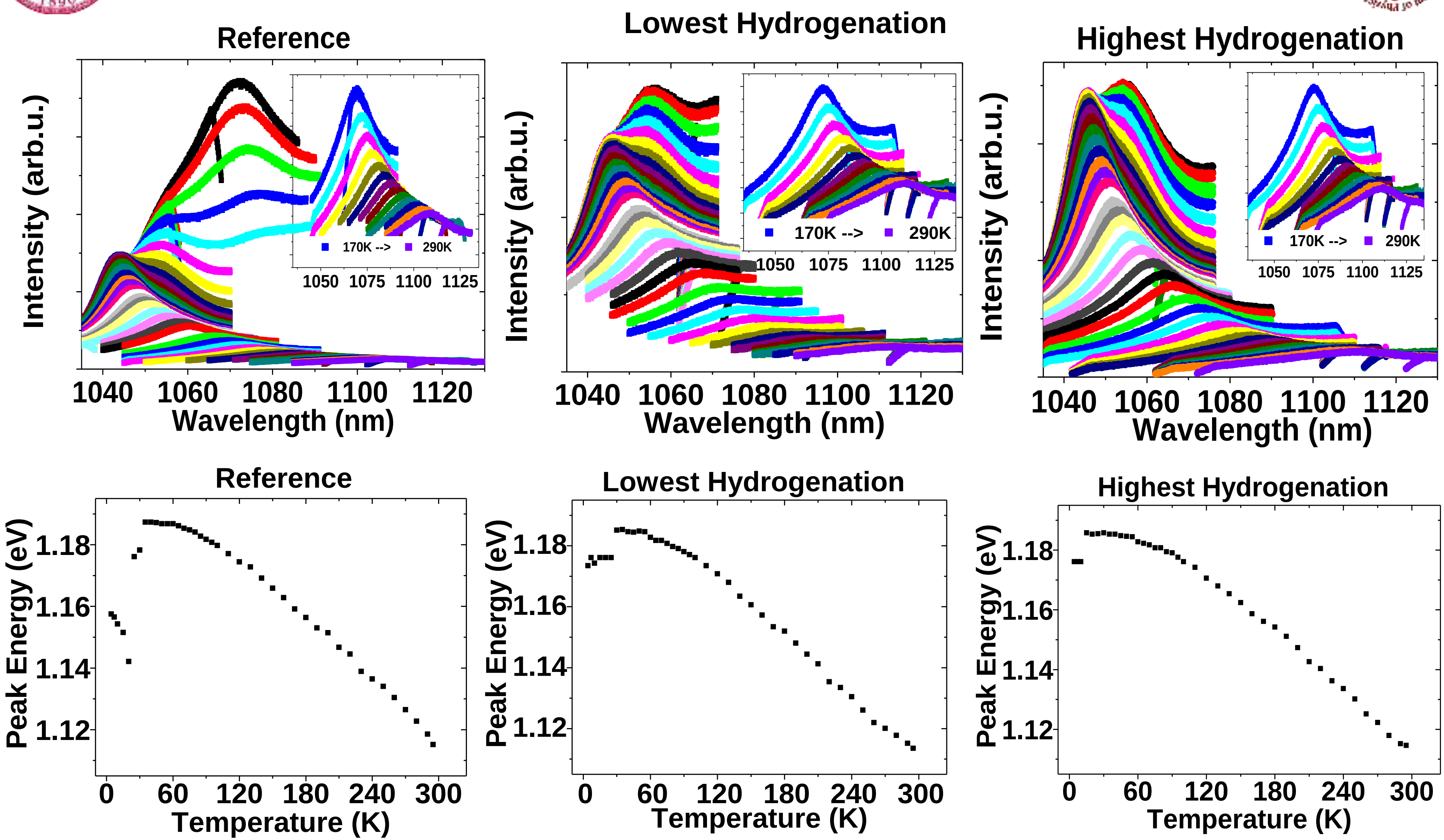




- UV-activated hydrogenation – Deuterium based
  - Typical 100 °C – 350 ° C
- Pressures ranging from 10^{-6} – 10^{5} Torr

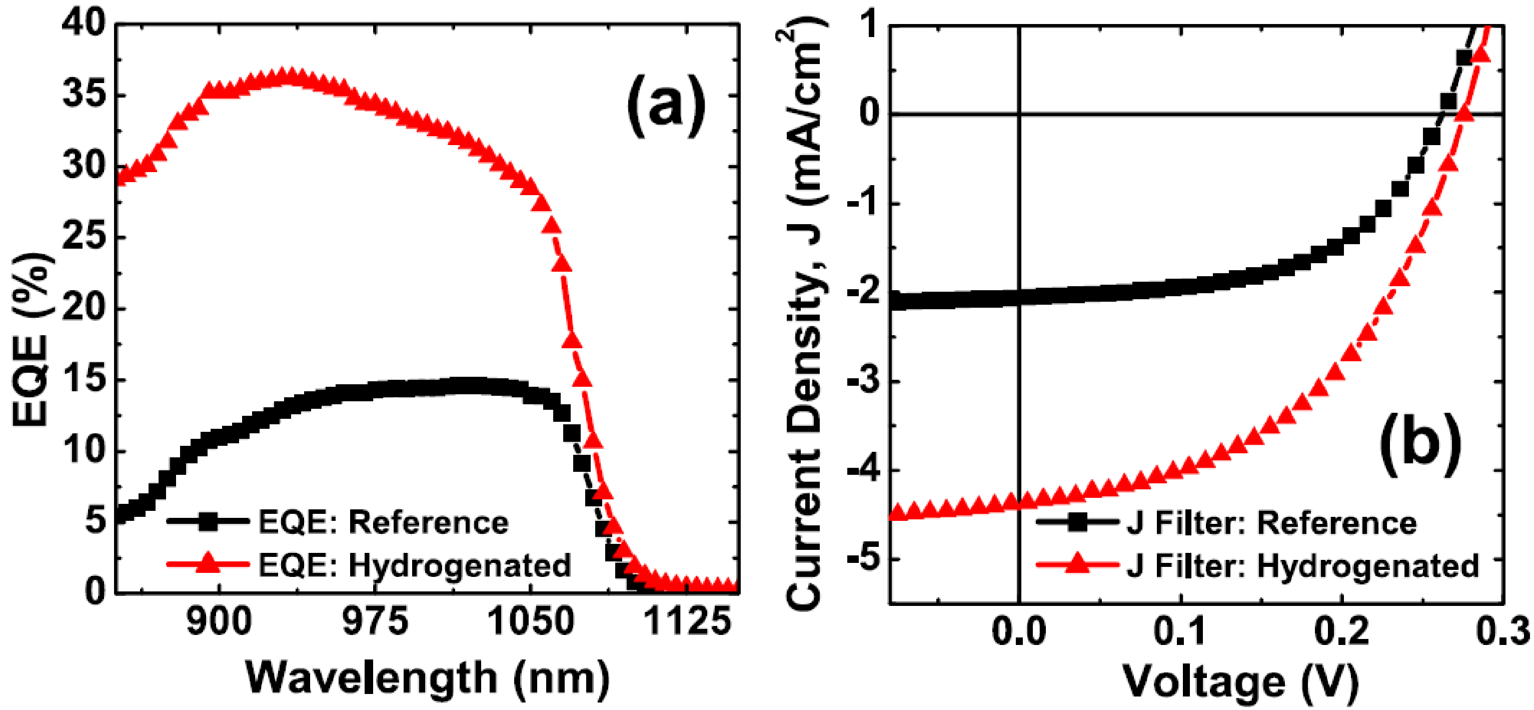
CRHEA

Passivation in Solar Cell



Proc. 40th IEEE PV Specialists, Denver 2014

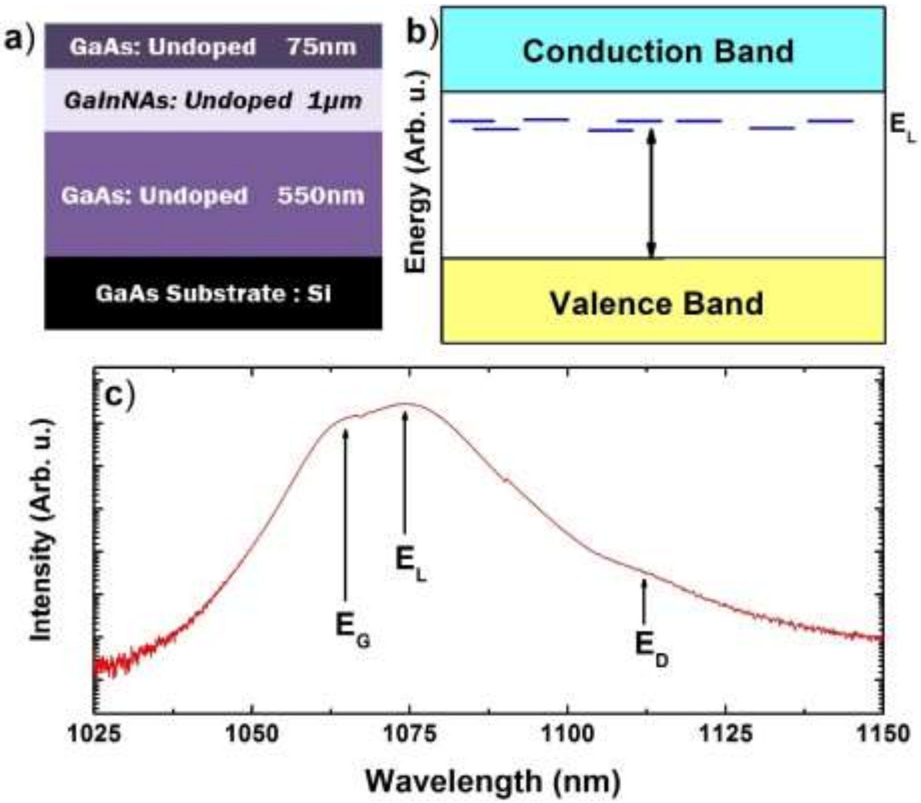
Solar Cell Characterization



- **Increase in performance of the solar cell after hydrogenation**
- **No visible effect on the substitutional Nitrogen – *selective passivation***

Fukuda *et al*. *Applied Physics Letters* **106**, 141904 (2015)

Samples Used



-Bulk $Ga_{0.91}In_{0.09}N_{0.028}As_{0.972}$ grown via MBE using RF plasma source for nitrogen

-annealed at 800°C for 30s

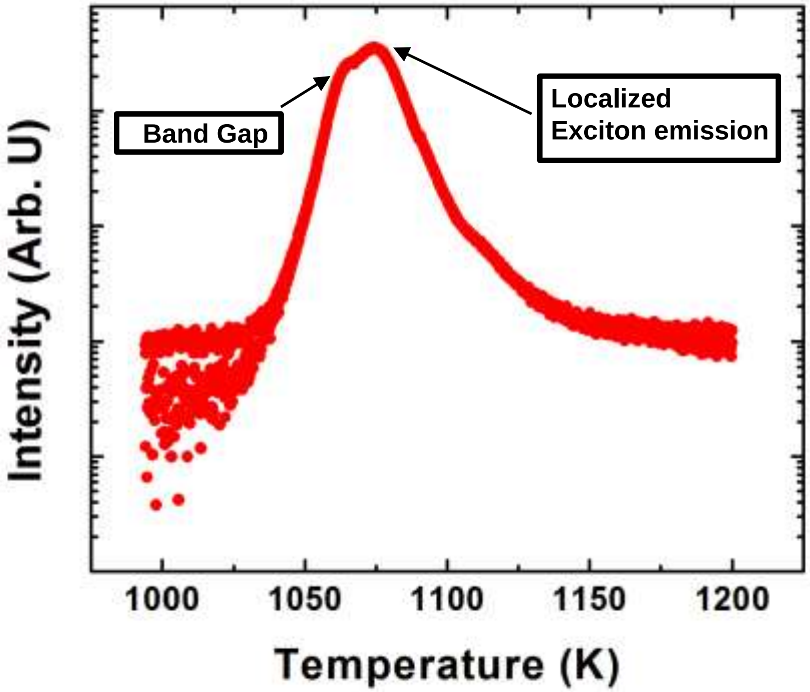
UV-Activated hydrogenation, 2 μm penetration

Three samples:

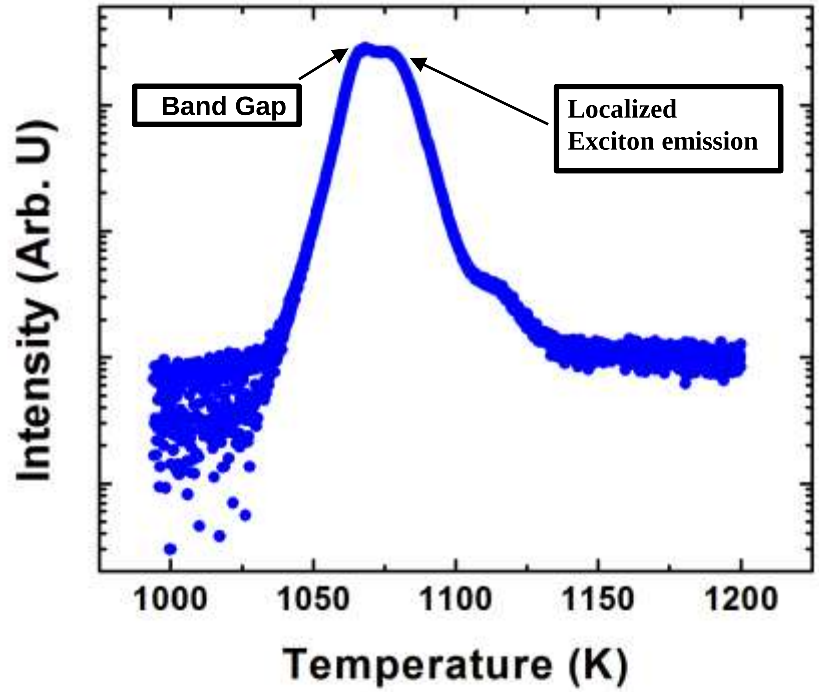
- Reference – Unhydrogenated
- #9 – Intermediate hydrogenation
- #8 – High hydrogenation

Hydrogenation of GaInNAs Mitigates Localization Effects, Retains Band Gap

Reference PL, 4K

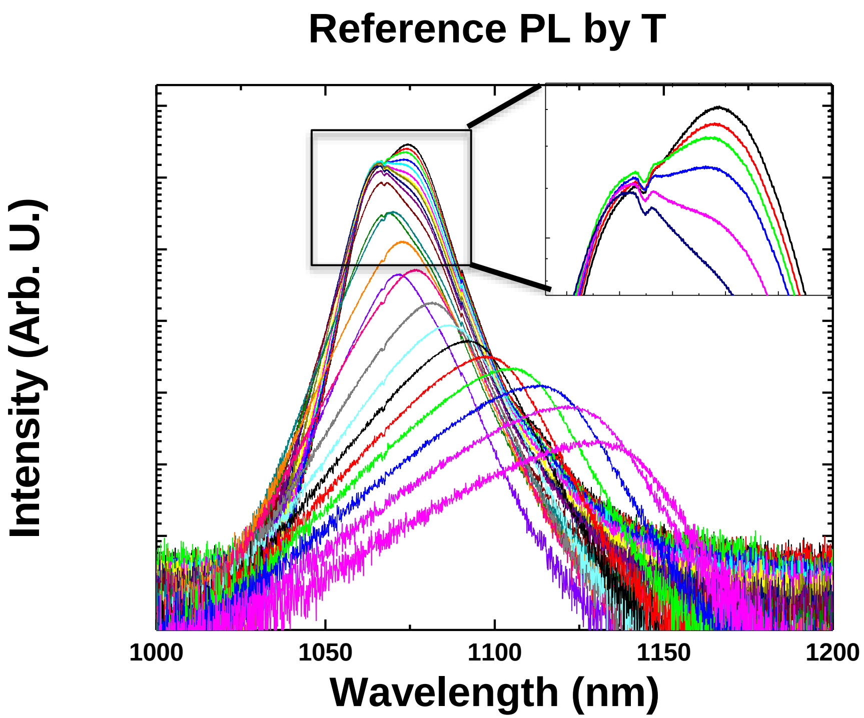


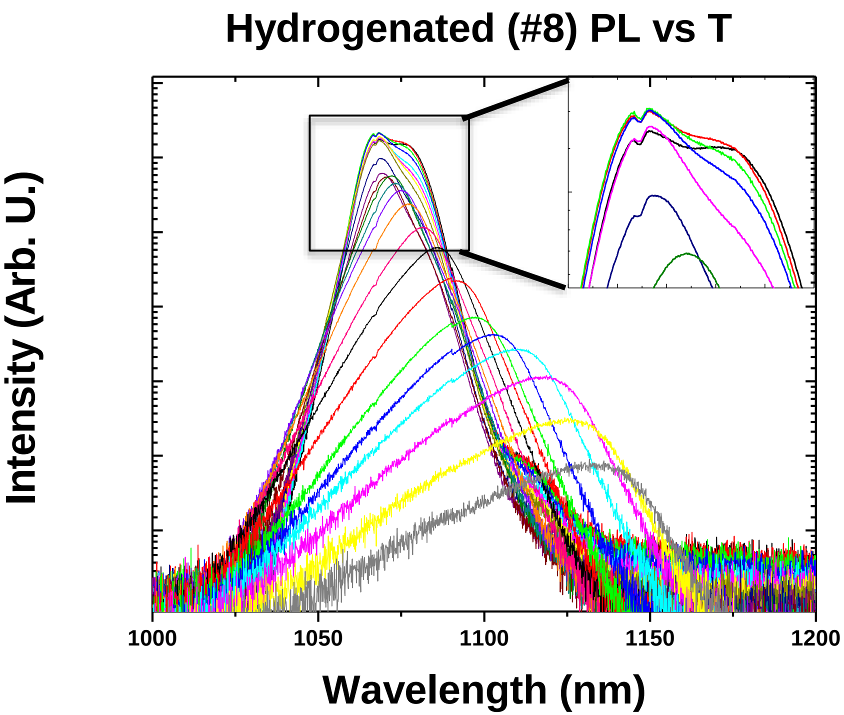
Hydrogenated Sample (#8), 4K



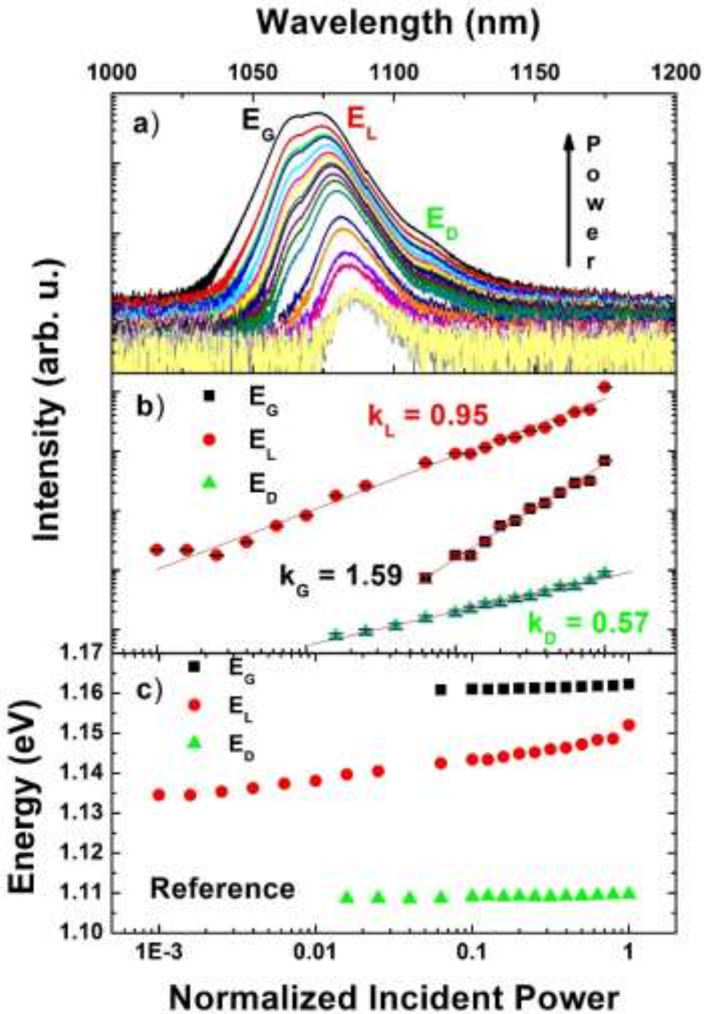
Reduction in intensity of low-energy “shoulder”

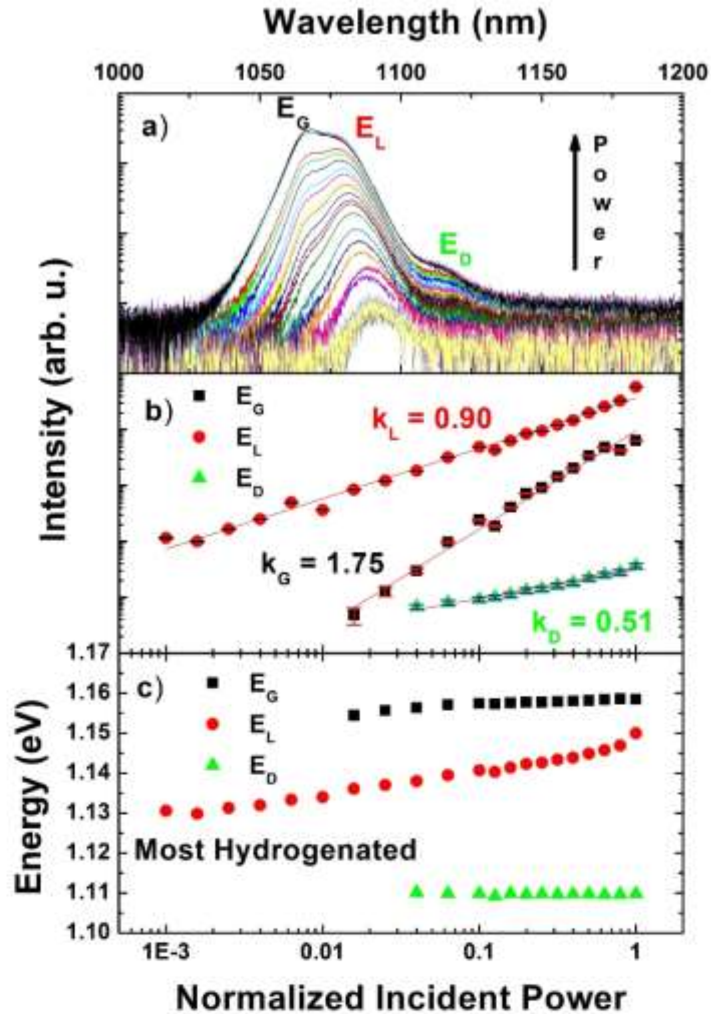
Hydrogenation of GaInNAs Mitigates Localization Effects, Retains Band Gap





Peak now has reduced ‘s-shape’ with temperature





•Individual Peaks E_G, E_L, and E_D are tracked and intensities are fitted

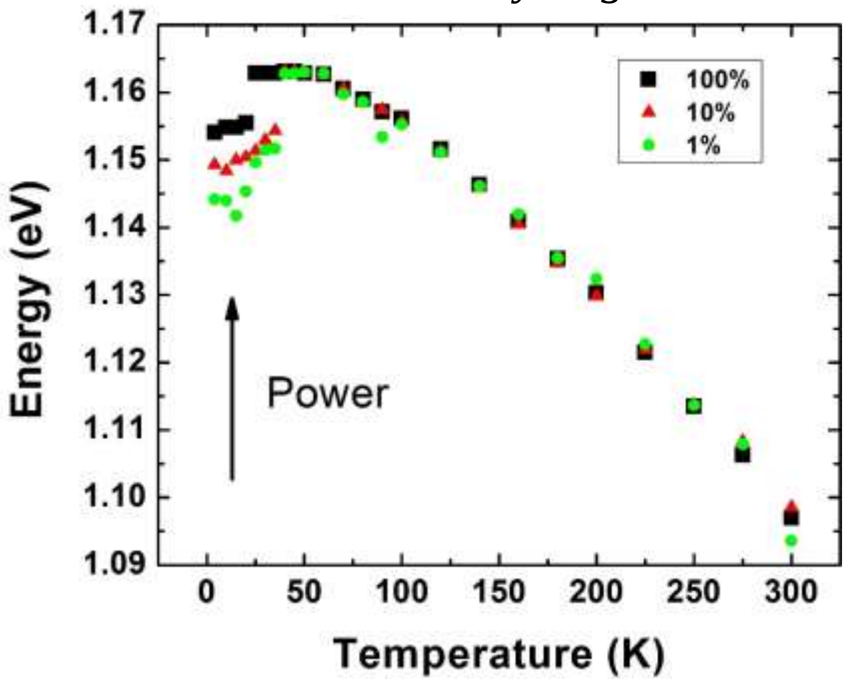
•k($I \alpha P^k$)

•k < 1 - Defect/localized states

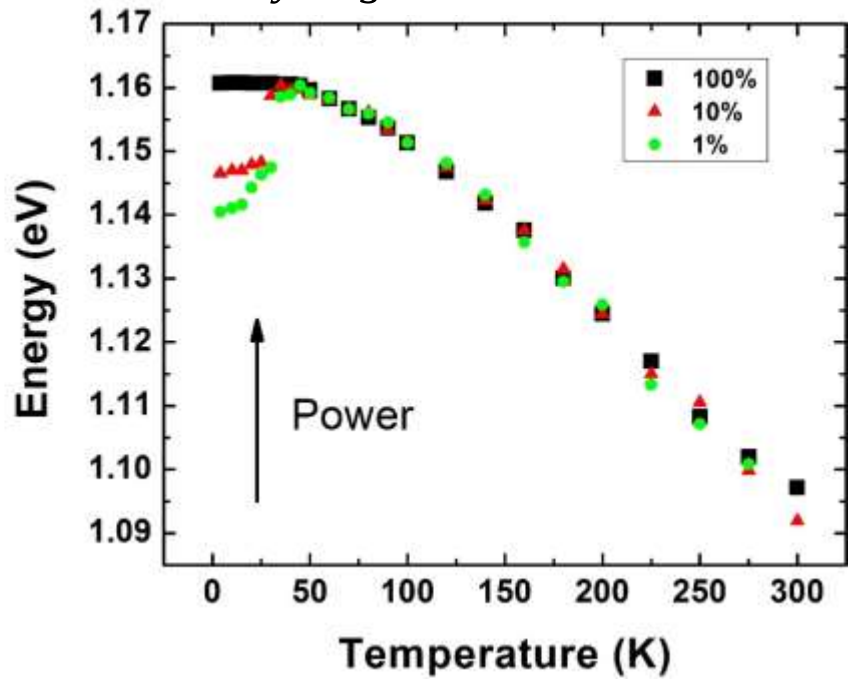
•1 < k < 2 - Band to band recombination

Selective Passivation: Effect of excitation intensity

Reference - *unhydrogenated*

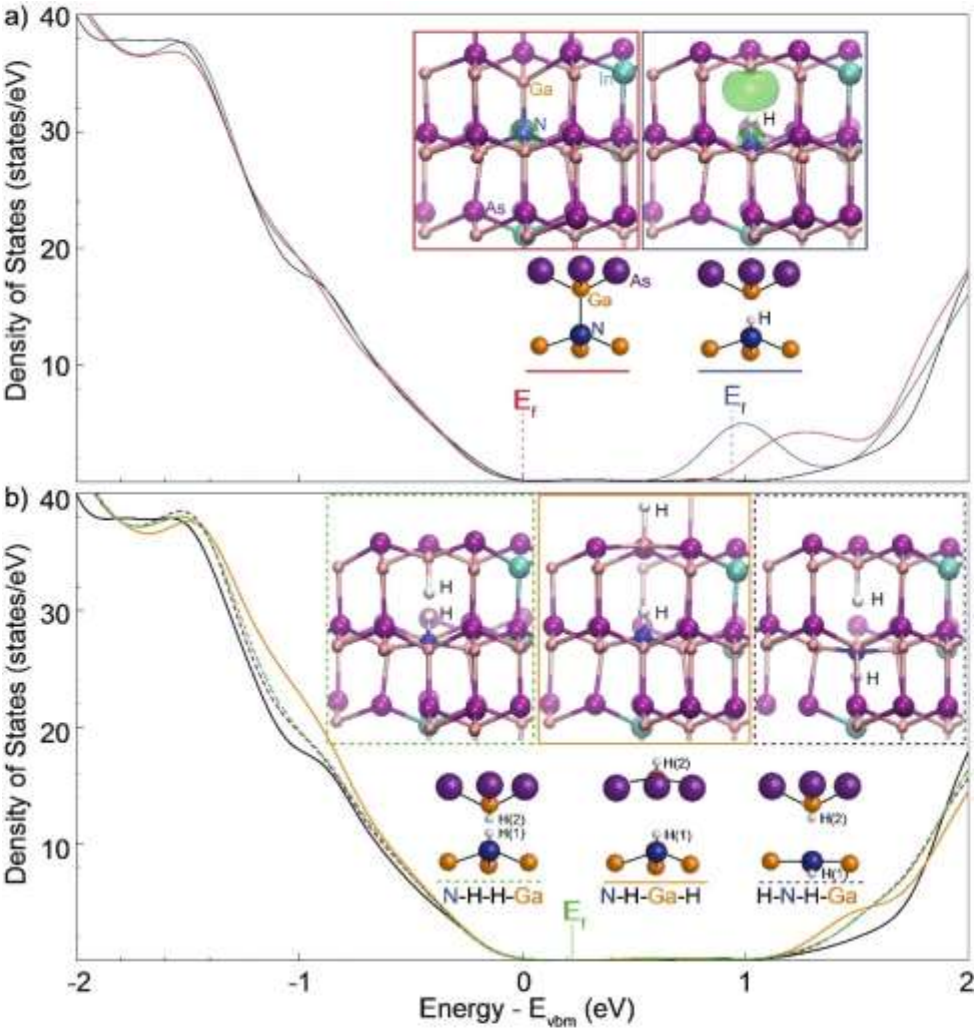


Hydrogenated – 1 x10^{15} cm^{-2}



Acknowledgement: Joseph Tischler and Chase Ellis

Density Functional Theory Results



- Supercell of 64 atoms used
  - 29 Ga, 32 As, 3 In
  - 1 N replaces an As atom for GaInNAs, giving 3% Nitrogen

- As Hydrogen concentration increases Ga-H_2-N complexes form. The feature related to nitrogen is pushed into the continuum. However the scattering center still remains.

Acknowledgement: Dr. Bin Wang – CBME, University of Oklahoma

Further Testing of Samples is Needed

- Annealing at different temperatures breaks certain N-H complexes, may be used to identify hydrogenation type
- Hall measurements will more directly ascertain effects of centers on carriers
- Thermopower measurements will qualitatively ascertain degree of doping change due to hydrogenation
- Transport Measurements
- Electrical Characterization - DLTS

Summary

- The hydrogenated samples exhibit lessened effects of localization centers while retaining substitutional nitrogen
- Further studies will be conducted to verify which N-H complexes are forming and to analyze their effect on the band structure and carriers.

Acknowledgements

OCAST OARS 12.2-040

DFT calculations performed at OSCER at the University of Oklahoma

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