Oxygen DX center in $In_{0.17}Al_{0.83}N$: Nonradiative recombination and persistent photoconductivity

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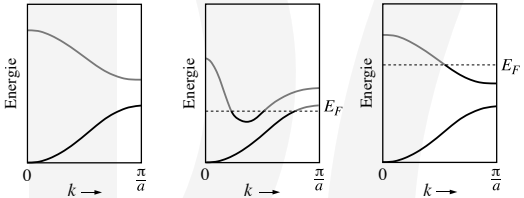
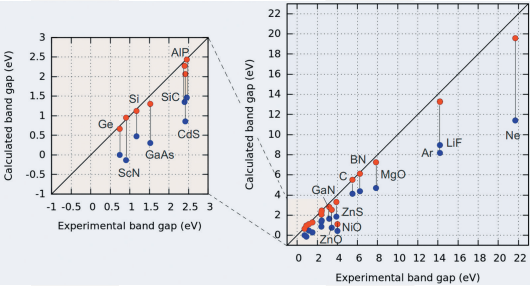
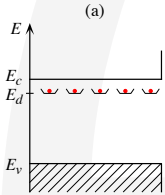
Metals, semiconductors and insulators

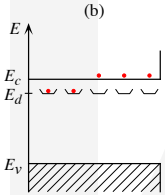


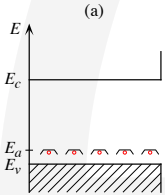
One of the major deficiencies of DFT is the underestimation of E_g when using local and semi-local functionals!

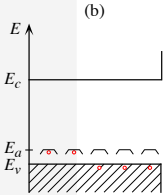


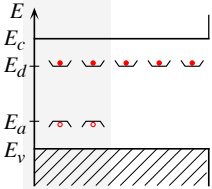
Defects and doping



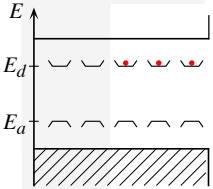








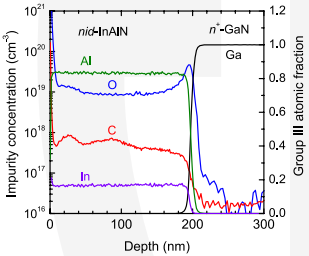
(a)

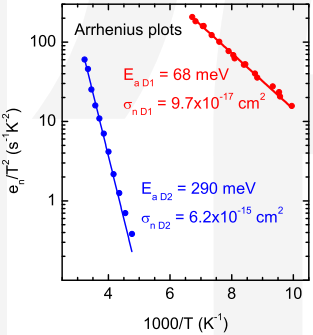


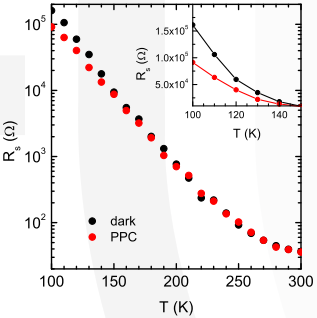
(b)

Defects in $In_{0.17}Al_{0.83}N$

Py *et al.*, Phys. Rev. B **90**, 115208 (2014)

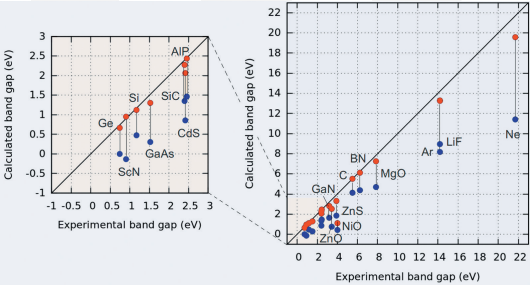


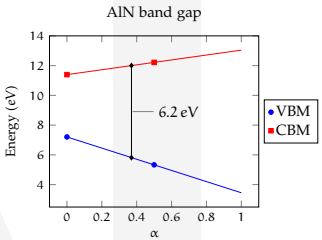


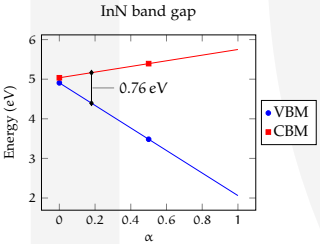


What is going on?

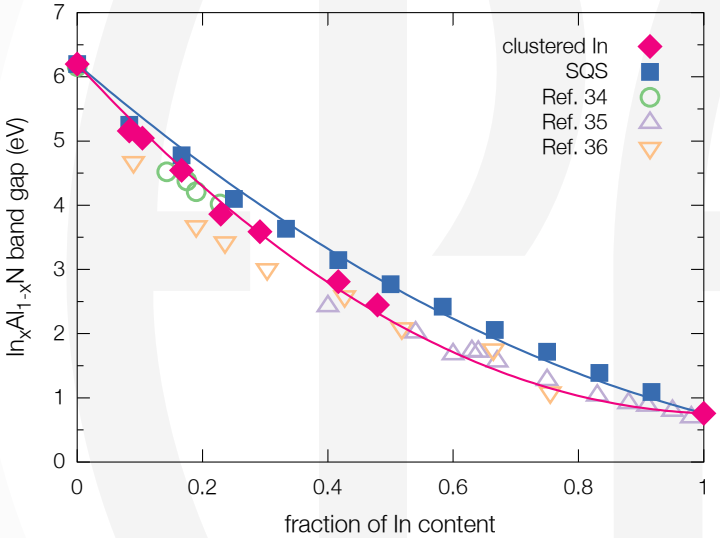
Addressing the band gap problem

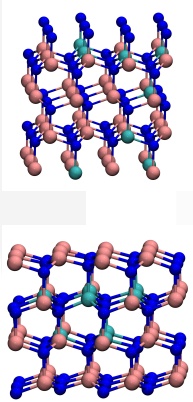






Structural model for $In_{0.17}Al_{0.83}N$

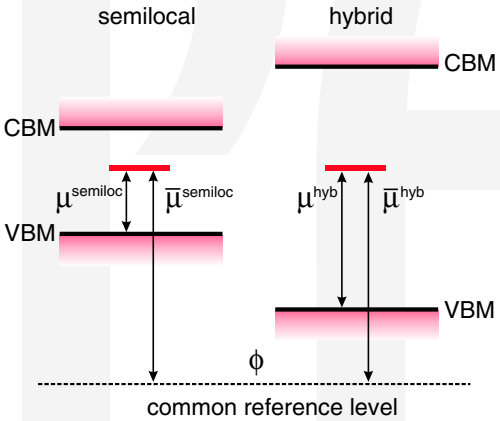




$b_{SQS} = 2.93\,\text{eV}$ $\quad b_{CS} = 5.2\,\text{eV}$ $\quad b_{exp} \sim 6\,\text{eV}$

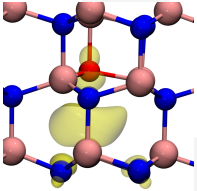
Formation energy from first principles

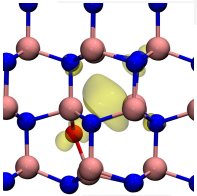
$$E_f[X^q] = E_{\text{tot}}[X^q] - E_{\text{tot}}[\text{bulk}] - \sum_i n_i \mu_i + q(E_v + \mu_e) + E^q_{\text{corr}}$$

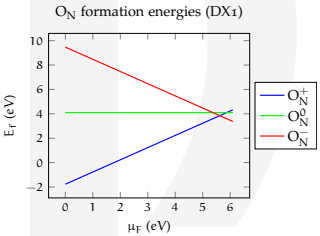


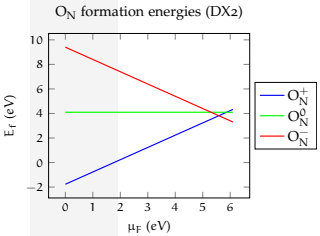
A. Alkauskas, P. Broqvist and A. Pasquarello, *Phys. Rev. Lett* **101**, 046405 (2008)

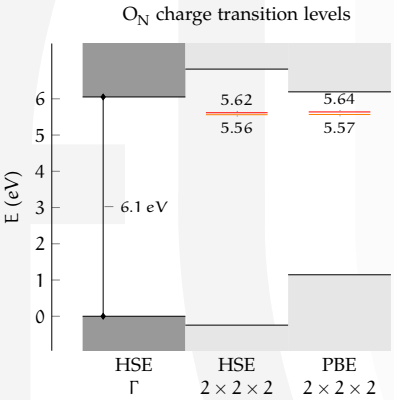
Benchmark: DX center in AlN



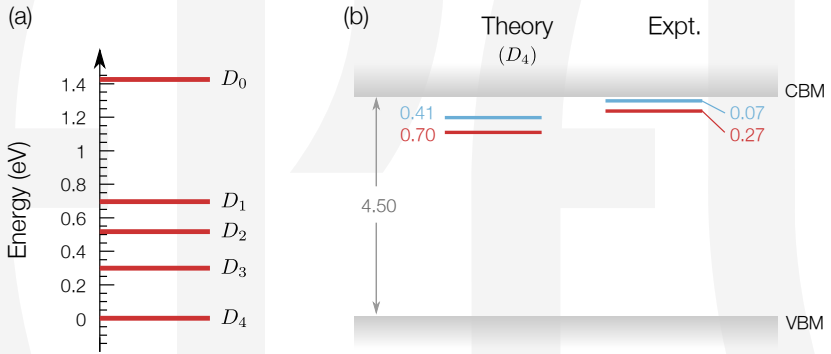




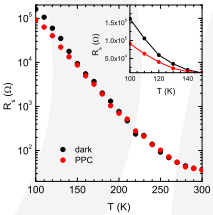


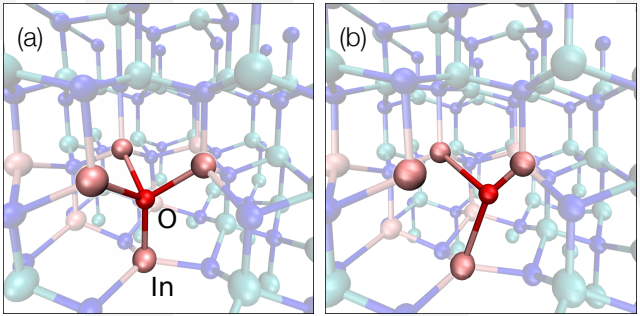


Formation energy and charge transition levels

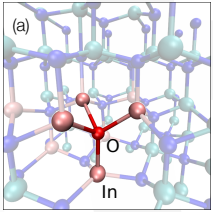


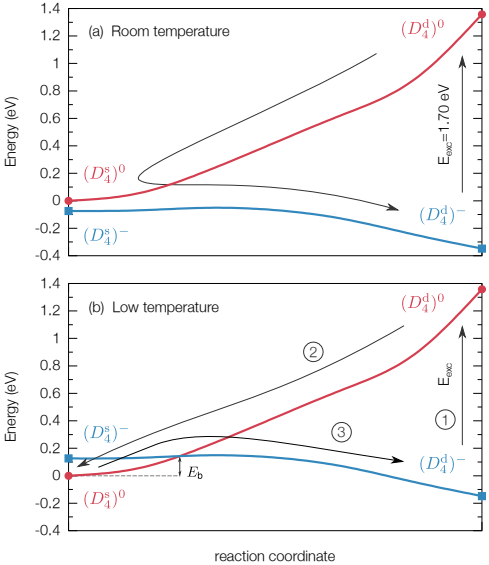
DX center

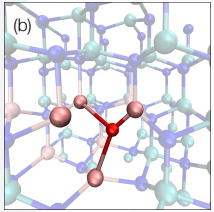

10^5
10^4
10^3
10^2
R_s (Ω)
100
150
200
250
300
T (K)
dark
PPC
$1.5x10^3$
$1.0x10^3$
$5.0x10^2$
R_s (Ω)
100
120
140
T (K)


(a)
O
In
(b)

PPC effects


(a)
O
In


(a) Room temperature
$(D_4^d)^0$
$(D_4^s)^0$
$(D_4^d)^-$
$(D_4^s)^-$
E_{exc}=1.70 eV
Energy (eV)
(b) Low temperature
$(D_4^d)^0$
$(D_4^s)^-$
$(D_4^d)^-$
$(D_4^s)^0$
E_b
E_{exc}
1
2
3
Energy (eV)
reaction coordinate


(b)

Conclusion

- In forms clusters in $In_{0.17}Al_{0.83}N$
- The oxygen impurity is more stable within In clusters
- Oxygen impurities forms DX centers in $In_{0.17}Al_{0.83}N$
- Oxygen impurities give rise to two CTL ($+/0$ and $0/-$) separated by 0.29 eV
- Oxygen is responsible to PPC effects at low temperature

Out calculations are in good agreement with experimental observation. We can assert that oxygen is the impurity responsible of PPC effects at low temperature and giving rise to the two observed CTL.

Acknowledgements

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