Dynamics of the V_N Negative U Center

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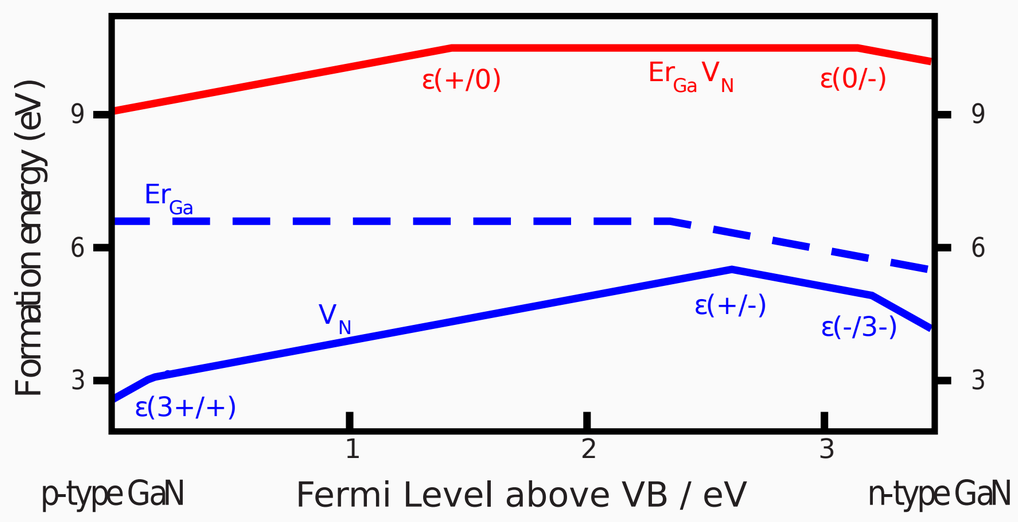
Motivation

The V_N defect in GaN has negative U behaviour in the regime of *p*-type doping. The centre is also considered to readily complex with substitutional rare earth impurities. Could these act as labels for the V_N centre behaviour?

Defect levels

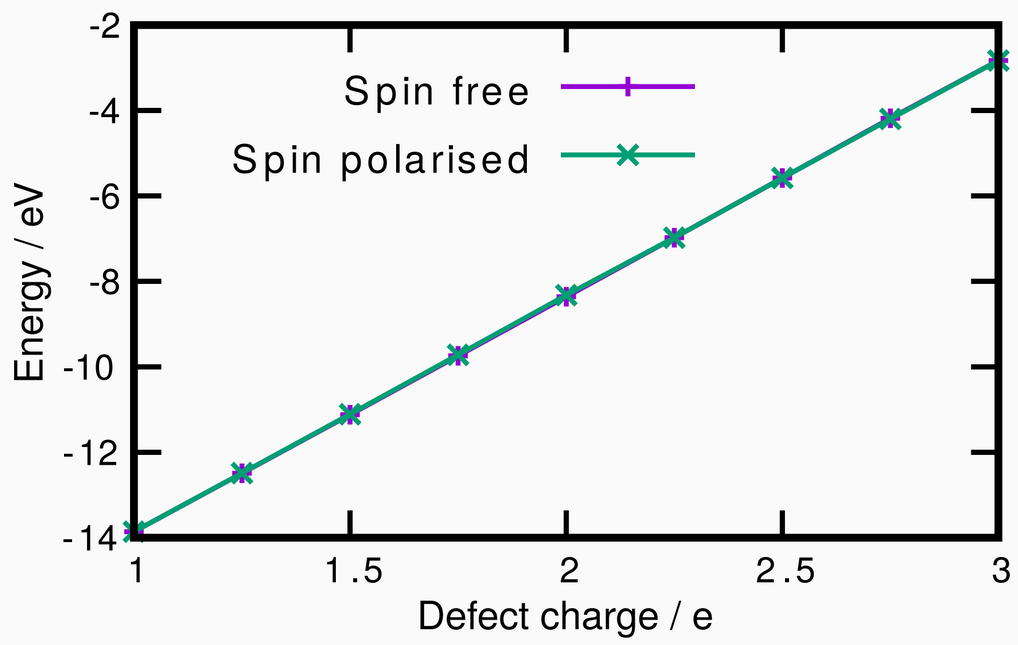


1. Equivalent to results of Sanna *et al.* Physical Rev. B **80** 104120 (2009).

Delocalisation error

A common issue in DFT and similar theories is the over-stabilisation of fractionally charged systems. This manifests as over-localisation of charge and the well known band gap error.

Fortunately, the energy of the V_N centre shows good linearity with respect to fractional charging:



Methodology

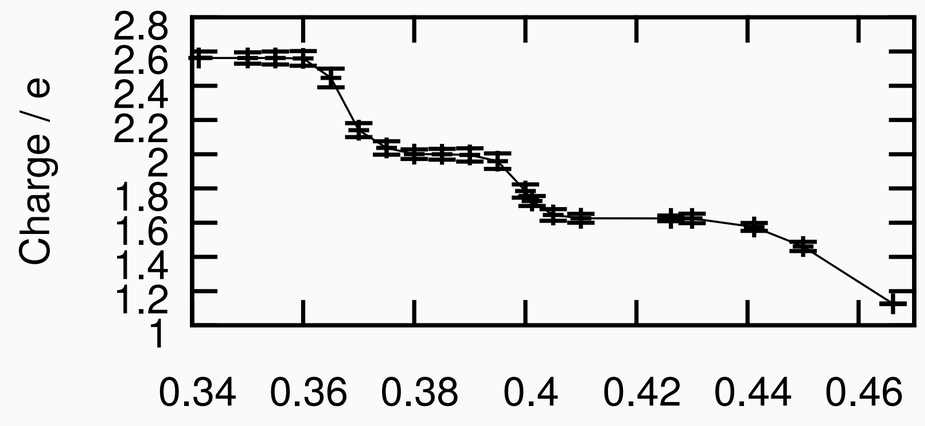
Self-consistent Density-Functional based Tight binding, supercell geometries.

- http://www.dftbplus.org
- rare-0-2 parameters [2]
- 4×4×4 Monkhorst-Pack *k*-points
- 400 atom unit cells (4×4×3 primitive Wurtzite cell)

2. Sanna *et al.* Status Solidi (c) **5** 2358 (2008).

Fixed Fermi level

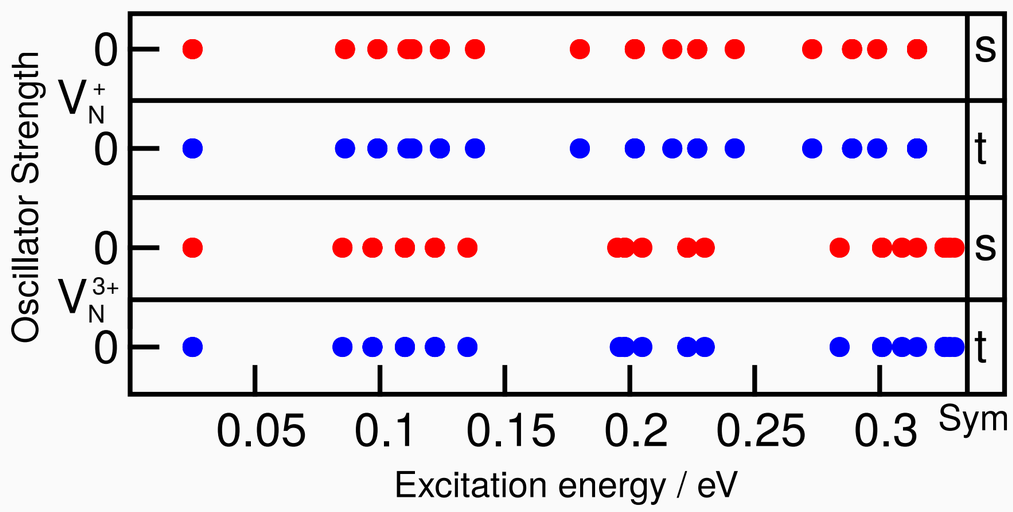
Aligning the band structure against shifts in potential, the total energy as a function of Fermi level shows indications of bi-stability on the order of ∼100 fs.



Average charge over molecular dynamics, ions and electron at 10 K, Nosé-Hoover thermostat and Fermi distribution of electron fillings.

Excited states

Time dependent DFTB calculations of the absorption transitions of V_N using Casida formalism.



Low energy excitations similar to the scale of E_F.

Summary

- Linear behaviour with charge – no evidence for lack of derivative discontinuity in this system.
- Low energy ‘dark’ excitations in the stable charge states.
- Evidence for multi-stable dynamics of V_N in the *p*-type region.