

# First-Principles Modelling of 2D Semiconductors

## NOWNANO Day Visit



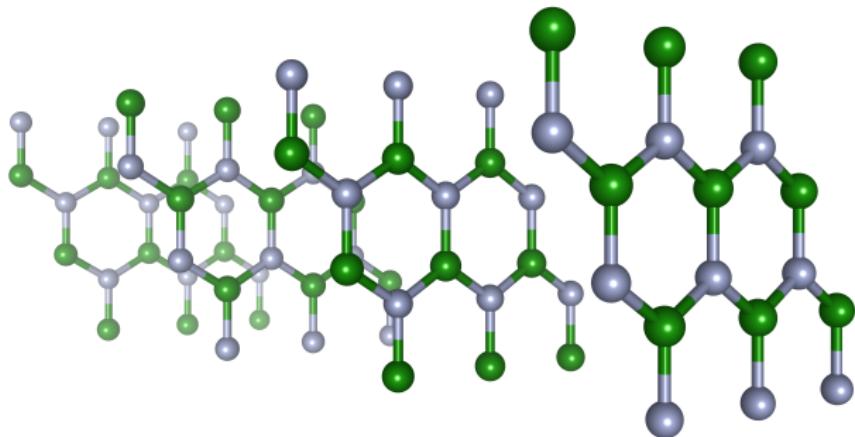
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Friday 11<sup>th</sup> November



# What do I do?

- ▶ Broadly speaking, I use **advanced electronic structure methods** to gain insight into the electronic<sup>1</sup> properties of materials.



**Figure 1:** Hexagonal Boron Nitride. If we didn't know about this material, how would we go about **determining** its properties?

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<sup>1</sup>or optoelectronic, or structural, or all.

# Why do I do it?

- ▶ We *know* existing alternative approaches are **deficient**.
- ▶ We **don't** always have the experimental capability to study a certain material in a certain environment.
- ▶ I believe that we should be capable of answering: "Why does material X have property Y". There is merit in **knowing**.

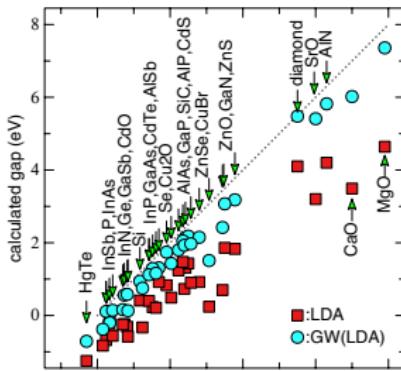


Figure 2: Bandgap problem of DFT (*and GW..?*)<sup>2</sup>.

<sup>2</sup>van Schilfgaarde, *et al.*, PRL 96, 2006.

# How do I do it?

- ▶ **Quantum Monte Carlo** : we use random sampling techniques to approximately solve the **full** many-electron Schrödinger equation.
- ▶ **Density Functional Theory** : despite its faults, DFT is still an immensely successful theory. If you know *nothing* about a system, DFT is worth using.



Lancaster  
University

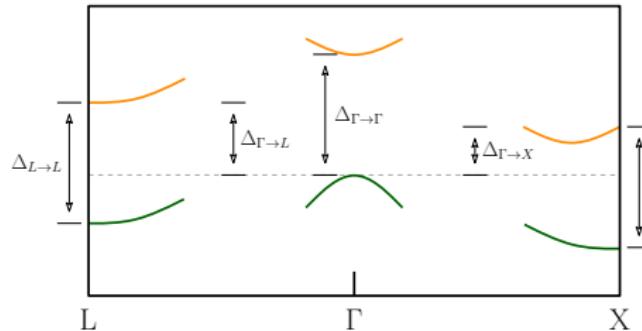


User	Total	Summary
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prdatlas015	809	: 809x1
huntr3	336	: 1x80 2x128
pltlhcbo16	322	: 322x1
pltatlas007	317	: 317x1
drummonn	288	: 1x128 1x160
fayon	176	: 1x16 1x64 1x96
famili	112	: 1x32 1x80

**Figure 3:** At any one time, I am running calculations on around 700+ HPC cores, usually  $\sim 350$  here on **HEC** and more on the **N8 HPC**.

# Examples of my research

- ▶ Lots of time recently on calculating **band gaps** for solids.



- ▶ Some results :

Gap	DMC	Expt. <sup>3</sup>
$\Delta_{\Gamma \rightarrow \Gamma}$	3.57(4) eV	3.4 eV
$\Delta_{\Gamma \rightarrow X}$	1.24(4) eV	1.2 eV
$\Delta_{\Gamma \rightarrow L}$	2.39(4) eV	2.0 eV

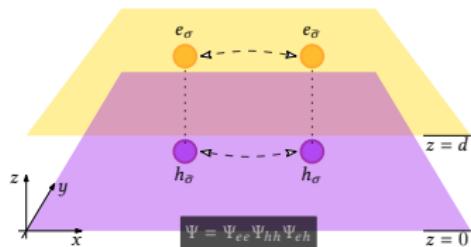
Figure 4: Schematic bandstructure of Si.

- ▶ Also studied hexagonal and cubic BN, bulk  $\alpha$ -quartz, several small molecules and dimers.

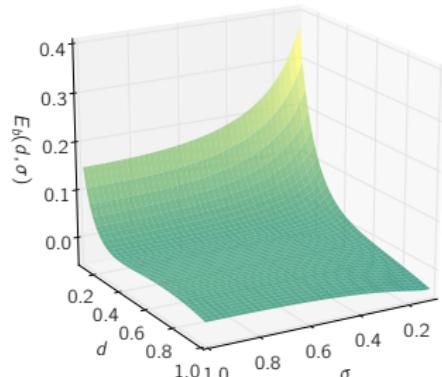
<sup>3</sup>Taken from ioffe.ru database - all at 300K.

## Examples cont.

- ▶ Not-so-recently, charge carrier complex binding in coupled quantum wells



**Figure 5:** Schematic of a biexciton in a CQW system.



**Figure 6:** QMC Binding energy of this biexciton.

# Summary

- ▶ I use highly accurate<sup>4</sup> electronic structure methods to (**hopefully**) obtain the right answers to **important** questions.
- ▶ I am a member of the ~1 in 9 "moved to Lancaster club" - and hence you can ask me general things if you are considering a move!

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<sup>4</sup>Systematically improvable, unbiased - but also very costly...