AIMPRO CONSORTIUM

UNIVERSITY OF NEWCASTLE UPON TYNE

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Ab initio simulation of covalent materials at Exeter, Newcastle & Sussex: computation with links to industry and experiment.

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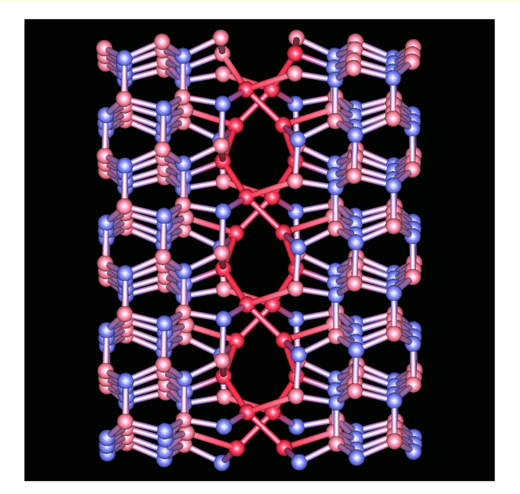
The consortium carries out modelling studies of covalently bonded materials with a view to supporting experimental and industrial groups. The code uses a **first–principles quantum–mechanical method** to explore the structural, chemical, mechanical, electronic, optical and magnetic properties of complex systems. **The complexity of these problems requires the UK HPC massive computational platforms.** We present here a selection of projects that are currently underway.

Diamond materials research

Collaboration with De Beers, groups in Novosibirsk, Aveiro and elsewhere resulting in a better understanding of the influence of defects on the **optical properties** of gem quality diamonds.

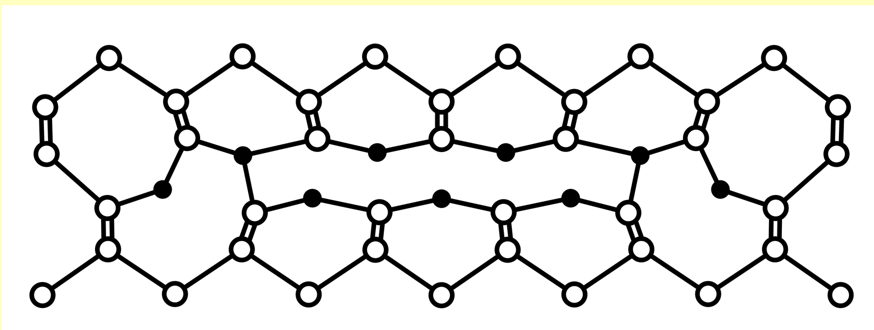
Dislocations in gallium nitride

Joint investigations with experimental physics at UMIST carrying out electron energy loss studies of extended defects in group III-nitride semiconductors. These materials have been singled out as providing **efficient blue lasers** and **bright white light emitters**, but with efficiencies limited by the presence of extended defects.



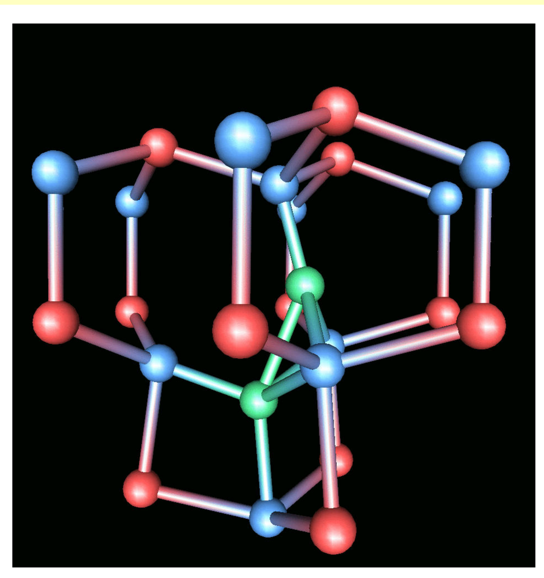
Gallium-core model of a threading screw dislocation in wurtzite gallium nitride

Oxygen in silicon



A collaboration with the experimental group at Lund (Sweden) into the nature of the **thermal donor** defect in silicon has lead to a model of the donor, shown above (○ - Si, • - O), which agrees with their experimental results.

Doping gallium nitride



The properties of Be and other **shallow acceptors in gallium nitride** is studied in collaboration with the Helsinki Technical University. This work has lead to a reappraisal of the acceptor efficiency of Be.

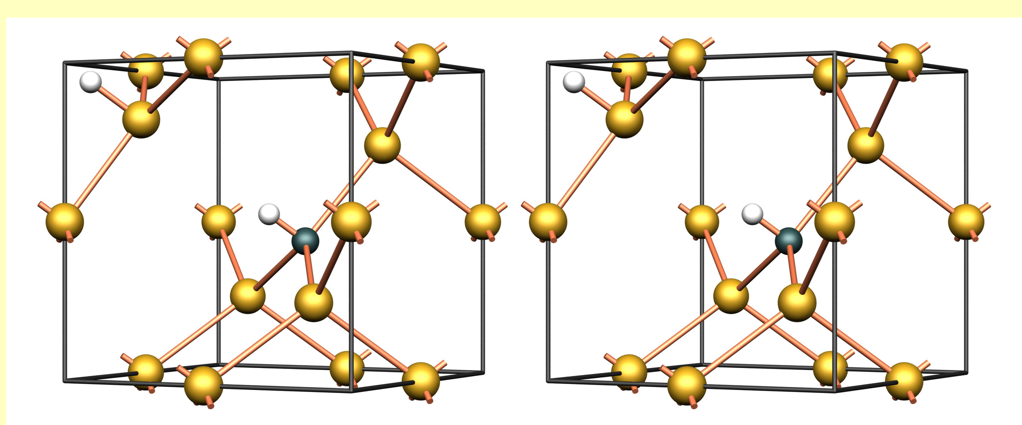
Beryllium pair defect at a gallium atom site in wurtzite gallium nitride (Ga; N; Be)

The nuclear power industry - BNFL

One of the most demanding challenges facing the nuclear industry is the long term storage of nuclear waste. In particular, graphite which has been irradiated at low temperatures might contain substantial amounts of energy which could pose a problem if released inadvertantly. First principles modelling of irradiation defects underpin existing phenomenological models of this 'Wigner energy' and give the industry, and its regulators, confidence in handling and disposing of this graphite safely.

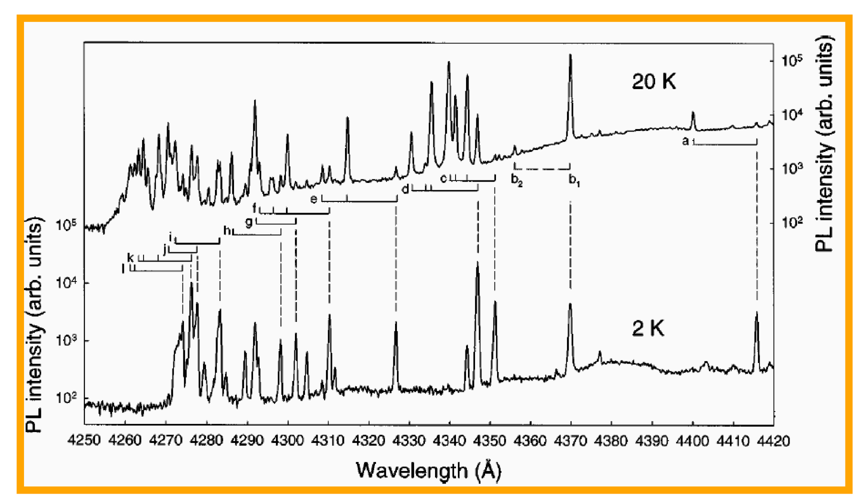
CSAR

Carbon and hydrogen in silicon



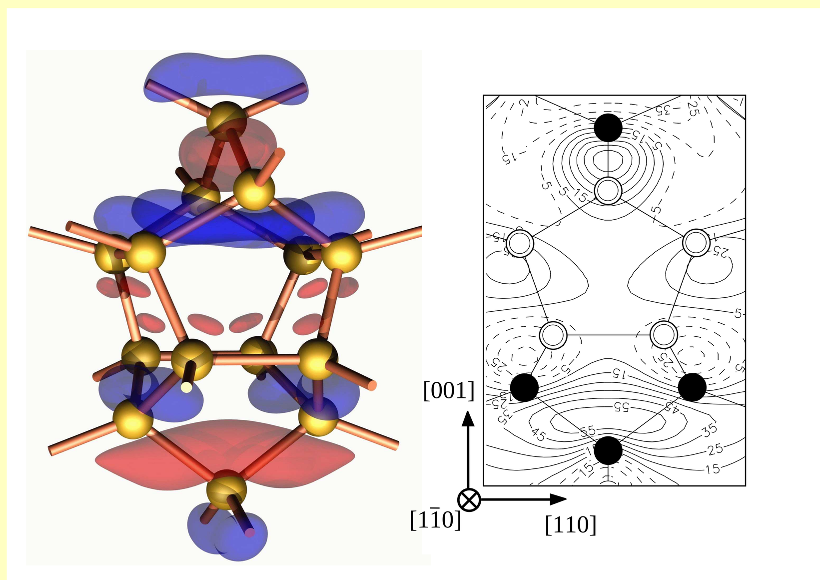
Collaborative work with the Department of Electronics at UMIST on the properties of hydrogen in silicon and specifically its interaction with carbon has lead to new findings regarding **traps for hydrogen** in the material.

Silicon carbide anti-sites



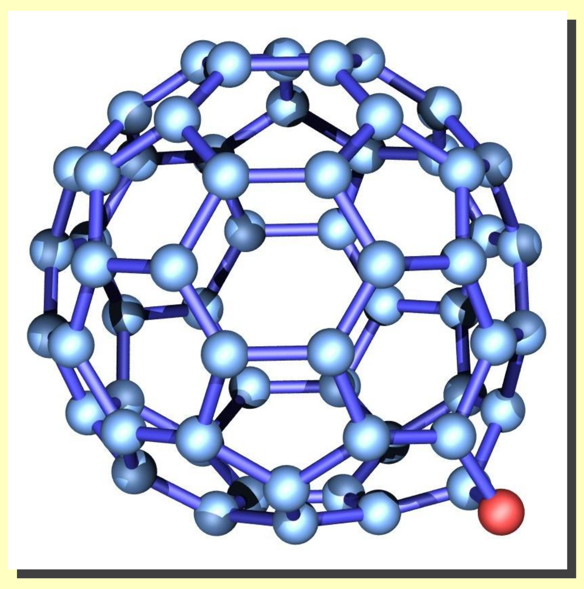
Silicon carbide is being developed as a **high temperature electronics material**. An unusual feature is the creation of defects giving 40 luminescent lines within a 0.1 eV interval (above) when the material is irradiated. Collaborative work with Bristol University has lead to a model for these centres based on an anti-site defect where as silicon atom occupies a carbon site.

Self-interstitial aggregates in silicon



There is intense interest in the properties of multi-interstitial centres in silicon formed after **ion-implantation**. We have recently succeeded in identifying two such aggregates, one of which is shown above, giving rise to prominent optical emissions. The work is carried out in association with experimental groups at King's College London and Brunel University.

Nanotechnology



The C_{61} molecule

Fullerenes and nanotubes feature among the most exciting new molecules which have **applications in nanotechnology**. Recent work has highlighted the importance of interstitials in allowing atomic reconstructions, important in achieving the stable icosahedral symmetry for the fullerenes and in different chiralities for the nanotubes.

Prestigious Publications

1. *Dislocation related photoluminescence in Si*, AT Blumenau, R Jones, S Öberg, PR Briddon and Th Frauenheim, Physical Review Letters, in press.
2. *Hydrogen interactions with dislocations in Si*, CP Ewels, S Leoni, MI Heggie, P Jemmer, E Hernandez, R Jones and PR Briddon, Physical Review Letters **84**, 690 (2000)
3. *Calculations of Electrical Levels of Deep Centers: Application to Au-H and Ag-H Defects in Silicon*, A Resende, R Jones, S Öberg and PR Briddon, Physical Review Letters **82**, 2111 (1999)
4. *First stage of oxygen aggregation in silicon: the oxygen dimer*, S Öberg, CP Ewels, R Jones, T Hallberg, JL Lindström, LI Murin, PR Briddon, Physical Review Letters **81**, 2930 (1998)
5. *Effect of oxygen on the growth of $(1\bar{1}00)$ GaN surfaces: The formation of nanopipes* J Elsner, R Jones, M Haugk, R Gutierrez, Th Frauenheim, MI Heggie, S Öberg and PR Briddon Applied Physics Letters **73**, 3530 (1998)
6. *Di-carbon defects in annealed highly doped GaAs*, J Wagner, Newman, BR Davidson, SP Westwater, TJ Bullough, TB Joyce, CD Latham, R Jones and S Öberg, Physical Review Letters **78**, 74 (1997)
7. *Theory of threading edge and screw dislocations in GaN*, J Elsner, R Jones, PK Sitch, Th Frauenheim, MI Heggie, S Öberg and PR Briddon, Physical Review Letters **79**, 3672 (1997)
8. *Auto-catalysis during fullerene growth*, BR Eggen, MI Heggie, G Jungnickel, CD Latham, R Jones and PR Briddon, Science **272**, 87 (1996)
9. *Interstitial-Carbon Hydrogen Interaction in Silicon*, AN Safonov, EC Lightowlers, G Davies, P Leary, R Jones and S Öberg, Physical Review Letters **77**, 4812 (1996)
10. *Shallow Thermal Donor Defects in Silicon*, CP Ewels, R Jones, S Öberg, J Miro and P Deák, Physical Review Letters **77**, 865 (1996)
11. *The twelve line 1.682 eV luminescent center in diamond and the vacancy-silicon complex*, JP Goss, R Jones, SJ Breuer, PR Briddon and S Öberg, Physical Review Letters, **77**, 3041 (1996)
12. *Limitations to n-type doping in diamond: the phosphorus-vacancy complex*, R Jones, JE Lowther and J Goss, Applied Physics Letters **69**, 2489 (1996)
13. *Theory of nickel and nickel-hydrogen complexes in silicon*, R Jones, S Öberg, J Goss, PR Briddon and A Resende, Physical Review Letters **75**, 2734 (1995)
14. *Identification of the Dominant Nitrogen Defect in Silicon*, R Jones, S Öberg, F Berg Rasmussen and B Bech Nielsen, Physical Review Letters **72**, 1882 (1994)
15. *$H, P^0 \rightarrow H, P^+$ transitions: A new look at donor-hydrogen pairs in Si*, SK Estreicher and R Jones, Applied Physics Letters **64**, 1670 (1994)
16. *The Structures of Dislocations in GaAs and their Modification by Impurities*, P Sitch, R Jones, S Öberg and MI Heggie, Physical Review B, Rapid Communication **50**, 17717 (1994)
17. *The H_2^* Defect in Crystalline Silicon*, JD Holbech, B Bech Nielsen, R Jones, P Sitch and S Öberg, Physical Review Letters **71**, 875 (1993)
18. *A Molecular Water Pump in Quartz Dislocations*, MI Heggie, Nature **355**, 337 (1992)
19. *Oxygen Frustration and the Interstitial Carbon-Oxygen Complex in Silicon*, R Jones and S Öberg, Physical Review Letters **68**, 86 (1992)
20. *Stable and Metastable States of $C_{60}H$: Buckminsterfullerene Monohydride*, SK Estreicher, CD Latham, MI Heggie, R Jones and S Öberg, Chemical Physics Letters **196**, 311 (1992)
21. *Multiple Charge States of Substitutional Oxygen in Gallium Arsenide*, R Jones and S Öberg, Physical Review Letters **69**, 136-39, (1992)
22. *Structure and Dynamics of the DX centre in GaAs:Si*, R Jones and S Öberg, Physical Review B, Rapid Communication **44**, 3407 (1991)
23. *Ab Initio Calculations on the Passivation of Shallow Impurities in GaAs*, PR Briddon and R Jones, Physical Review Letters **64**, 2535 (1990)