Computational Solid State Physics Research Group

Research Group Leader

Prof. Nithaya Chetty
BSc Hons (U. Natal), PhD (U. Illinois)
Office : Room 5-54 Natural Sciences Building NW1
Telephone: (012) 420-6204
Email: Nithaya.Chetty@up.ac.za

PhD Students

Mr. Richard Andrew
BSc Hons (UP), MSc (UP)
Richard.Andrew@up.ac.za

Mr. Gilbert Mashapa
BSc (Hons) U. Lim, MSc (U. Lim)
mmashapa@csir.co.za

Mr. Bongani Ngwenya
BSc Hons (UWC), MSc (UWC)
bongani.ngwenya@gmail.com

Mr. Edwin Mapasha
BSc Hons (U.Lim), MSc (UP)
sengere@webmail.co.za

Mr. Kingsley Obodo
BTech (NAU), MSc (AUST)
obodokingsley@gmail.com

MSc Students

Ms. Eva Khoza
BSc Hons(U.Limpopo)
khzeva1@gmail.com

Post-Doctoral & Research Fellow

Dr Trisha Salagaram
Post-Doctoral Fellow
trisha.salagaram@up.ac.za

Dr Aniekan Ukpong
Research Fellow
aniekan.ukpong@up.ac.za

Honours, Masters, Doctoral students and Postdoctoral fellows are welcome to join the Group. What interests and experiences do you need?

1. ***Quantum mechanics, solid state physics, statistical physics***
2. ***Passion for computing, use of the Linux operating system, graphical work preferably in an Open Source environment***

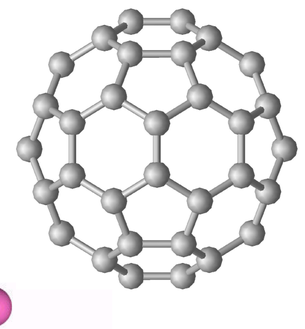
Theoretical Formalism

Density Functional Theory (Walter Kohn, Nobel Prize 1999)
Approximations for Exchange-Correlation Potential
Van der Waals interaction, DFT + Hubbard inter-action
Finite Temperature Quantum Molecular Dynamics
Approximate total energy methods

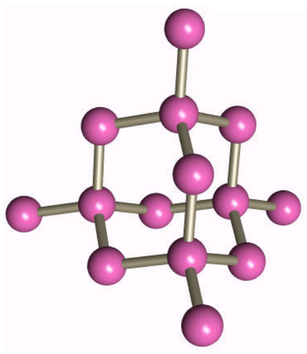
$$\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right]\Psi_i(r) = \varepsilon_i \Psi_i(r)$$

Computational Resources

Electronic Structure Programs
Vienna *Ab initio* Simulation Package (VASP)
Quantum Espresso (QE)
Brookhaven Electronic Structure (BEST)
Cambridge Atomic Simulation Total Energy Package (CASTEP)



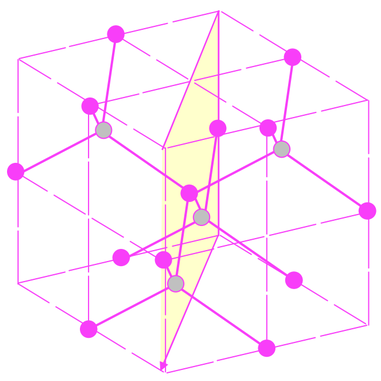
Hardware
Powerful desk computers
University of Pretoria Computational Cluster
Centre for High Performance Computing (CHPC)



$$U = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl}$$

Research Activities

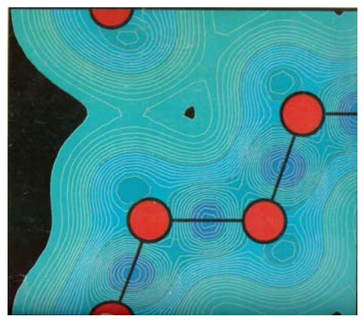
Graphene, Boronitrene
Adatoms, impurities, vacancies
Electronic Structure
Graphite and graphitic structures
Elastic properties
Bi-layers, multilayers



Silicon carbide
Elastic properties
Alloys of Si and C; search for stable structures
Finite temperature; Quasi harmonic approximation
Surfaces

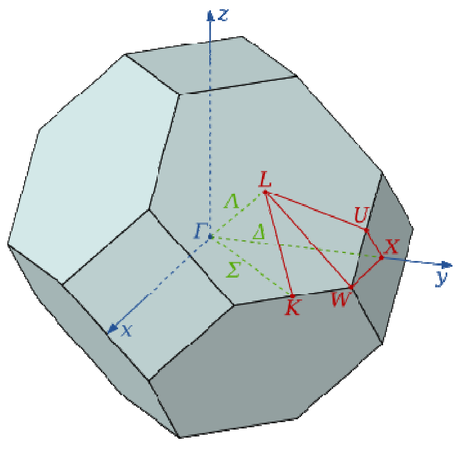
C and BN nanotubes
Substitutional impurities, vacancies
Changes of the electronic structure with doping
Effects of various forms of exchange-correlation potential

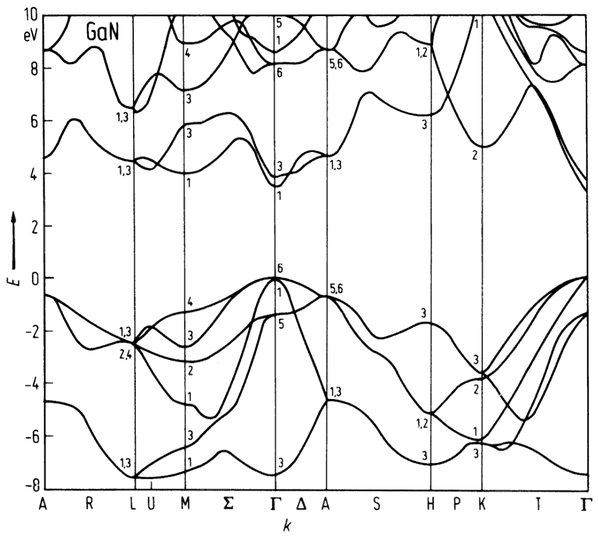
Finite temperature quantum molecular dynamics
SiC/Graphite interface
Born-Oppenheimer dynamics
Car-Parrinello dynamics



Alloys of Lanthanides and Actinides
Alloy formation with B, C, N, O and Ti
Defect studies
DFT + Hubbard
Quasi-harmonic approximation

Computational Physics Research
Translating research problems to computational problems in the class room
Quantum mechanics, statistical physics, classical mechanics, solid state physics
Fortran90, Easy Java Simulations





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