

PROFILE

Computational Solid State Physicist. Currently employed in developing the *Fireball* ab-initio molecular dynamics package. Employed in the Lewis Group at West Virginia University. An IRCSET Scholar.

EDUCATION**DUBLIN INSTITUTE OF TECHNOLOGY, PH.D. DEFENDED JUNE 10TH 2011.**

Project Title- "*Calculation of the electrical and optical properties of nanoscale systems*", with a particular focus on three systems: potassium overlayers on 3C-SiC(100), Mott-Hubbard transitions on the 3C SiC(111) and 6H SiC(0001) surfaces, and the In-Si(111) system and its so-called "quantum wire" characteristics.

Project includes the modification of the *Fireball* ab-initio molecular dynamics package to calculate unique spectra, such as the reflection anisotropy experimentally seen on the In-Si(111) surface. Other key aspects include: the investigation of the discrepancy between experimental and theoretical results for the 3C SiC(111) and 6H SiC(0001) surfaces, and evaluation of the behaviour of metallic overlayers on silicon and silicon carbide.

A major component of this study led to the development of a very strong collaboration with the Lewis Computational Solid State Physics group at West Virginia University. This has resulted in extended visits to the US to study advanced *computational physics* techniques.

DUBLIN INSTITUTE OF TECHNOLOGY, B.SC. (HONS)PHYSICS AND PHYSICS TECHNOLOGY, 2004. (ACHIEVED- FIRST CLASS HONOURS (G.P.A. > 3.5))

Core Modules included:

Electronics and Instrumentation, Lasers, Optical Communications and Other Applications, Radiation and Nuclear Physics, Electromagnetism, Quantum Physics of Solids, Computational Physics.

Final Project- Development of a CT Scanner for education purposes.

All Optional courses were studied, including:

Acoustics, Fluid Dynamics, Microwaves, Physics of Materials, Medical Physics, Applied Optical Spectroscopy, Digital Signal Processing

INSTITUTE OF TECHNOLOGY, TALLAGHT, DIPLOMA, INSTRUMENTATION AND APPLIED PHYSICS, 2002. (ACHIEVED- MERIT, GRADE 1 (3.5 > G.P.A. >2.75))

Course included Passive Electronic, Digital Electronics, Computational Physics, Instrumentation, Mathematics, Process Control, P.L.C. Programming, Materials Science
Final Project- Development of Voltage Controlled Musical Synthesizer from Passive Components.

INSTITUTE OF TECHNOLOGY, TALLAGHT, CERT. IN INSTRUMENTATION AND APPLIED PHYSICS, 2001. (ACHIEVED- DISTINCTION (G.P.A. >3.25))

Course included Introductory Biology & Chemistry, Maths, Electronics, Instrumentation, Computer Programming.

TERENURE COLLEGE, TERENURE, DUBLIN 6W.

Leaving Certificate, 1999

Mathematics, Physics, Chemistry, Irish, English, French, Social and Scientific Studies, Accounting.

TEACHING EXPERIENCE

WEST VIRGINIA UNIVERSITY.

Attend and present regular research reports. Weekly Post-Grad talks on subjects of interest. Delivered and received multiple classes on various topics within the Computational Physics regime, including: the McWEDA Approximation, Linear Density Approximation, the *Fireball* implementation of *ab-initio tight binding Molecular Dynamics*, and related topics.

Regularly assist undergrads in their studies in Computational and Solid State Physics.

Currently assist teaching a computing and robotics course for undergrad summer school, the *Moutaineer Area Robotics Team* (MARS).

Voluntarily tutored students in computational physics, and on their other physics related courses on a one to one basis.

DUBLIN INSTITUTE OF TECHNOLOGY

Delivered tutorials to second and third year physics students on entire prescribed coursework including: Optics and Electromagnetism, Mechanics, Relativity, Heat and Thermodynamics, Electronics and Semiconductors, Condensed Matter, Nuclear Physics, Vibrations and Waves.

Delivered "Labview" course to second year physics course. Labview is a G.U.I. based computer programming language. Redesigned and modernised the course content to reflect current technologies and software capabilities.

Supervised Labs in Physics first through third year. Also supervised laboratory work for non-traditional students.

Designed and maintained fourth year lab experiment based on computed tomography.

Tutored two students in physics under student retention programme.

Supervised a Spanish exchange student in coursework project required for bachelors' degree.

IDT LTD.,

Delivered regular tutorials and courses to dentists' on the subject of computed tomography (CT) and segmentation of CT studies, including planning of implant surgery using computer-aided techniques.

Hosted three training sessions (schools) in the Dublin Dental School and Hospital, Trinity College on surgical planning using computer aided techniques and CT.

Carried out regular on-site training days for newer employees in principles of 3D segmentation and basic CT technologies.

OTHER,

While working on undergraduate degree, tutored students in Mathematics and Physics for Leaving Certificate and Junior Certificate courses (High school level).

Tutored students from *University College, Dublin, Ireland* and *West Virginia University, US* in Physics and Mathematics at undergraduate level.

Active mentor of the high school robotics team Mountain Area Robotics Society (MARS). The team qualified for the World Championships 2010 in Atlanta Georgia.

RESEARCH EXPERIENCE

PH.D.

Computational Physics/Solid State Physics. Current projects are on soft-phonon transitions on the 3C-SiC(111) and 6H-SiC(0001) surfaces, as well as a paper on the K-3C-SiC (100) surface metallisation.

Very strong collaboration with the Lewis Computational Solid State Physics group in W.V.U.

Modernised and rewrote the current implementations of algorithms for the *Fireball* molecular dynamics code, specifically the *Create* program.

Developed new integration routine for *Fireball*, as well as the new neighbor-interactions code and overall revamp of older code. (see Employment section) .

Worked extensively on the In-Si(111) surface metallisation. Working in conjunction with the Lewis Group to develop a RAS spectrum of this surface using the newly rewritten code.

B.SC.

Final Project: development of a senior undergrad lab experiment to explain Computed Tomography. Included the design and build of apparatus as well as a software suite that would not only show how *Iterative Backprojection* worked, but also demonstrates how the computational back-end actually carries out the process.

Previous research projects included: Modelling of carbon nanotubes based on the chiral vector. This was part of the work required for an lecturers' Ph.D. and development of a music synthesiser via passive electronic components, which was modelled using the P-Spice software package.

I.D.T. LTD.,

Published report at the *Applied Physical Sciences in Medicine Conference in Galway in 2005* entitled "*Evaluation of Current Dental CT Technologies*". This report and subsequent presentation was based on study carried out on the request of the Managing Director.

Researched and developed computing technology in order to read older CT (known colloquially as "CAT Scan") media and transfer to newer format. This required learning how systems such as VAX were originally designed and coded, and in many cases simulating older environments so the media could be accessed.

TAX BACK INTERNATIONAL.,

Carried out study on basic V.A.T. (Value Added Tax) laws throughout Europe and the US as part of an in-house report, which was presented to the Managing Director in 2003.

Researched and reported on various international conferences. This assisted colleagues in the development of rapport and clientele.

EMPLOYMENT HISTORY

PH.D STUDENT, DUBLIN INSTITUTE OF TECHNOLOGY, IRELAND — 2004-PRESENT

Current employment, see Education and Research sections.

Duties include, but not limited to: Analytical and computational calculations of atomic systems via the use of the ab-initio DFT software package known as *Fireball*. Extensive revision of the *Fireball* code for modernisation and clarification purposes. Assisting researchers with the fundamental elements involved in Density Functional Theory and its use in the *Fireball* MD package. Bridging and enhancing possible collaborations both theoretical and experimental physics.

Prior to extended visits to W.V.U., responsibility in the *Nanophysics & Surfaces* lab in DIT was lab maintenance, including the ultra-high vacuum chamber and computational facilities.

PART TIME TUTOR, DUBLIN INSTITUTE OF TECHNOLOGY, IRELAND — 2004-2007

Rewrote and delivered Labview course for second year students 2005 - 2007.

Supervised undergrad labs first through third year in both Physics and Engineering.

Supervised and delivered classes designed for non-traditional students in Engineering.

Delivered tutorials across all aspects of second year physics course, see "Teaching" section.

Supported Computed Tomography (CT) fourth year lab which used the apparatus that was built as partial fulfillment of the requirements for my B.Sc.

IRISH EXECUTIVE, IDT LTD., LONDON, UK — 2004

Responsible for all Irish clients of U.K.-based medical physics company.

Held exclusive rights to Irish market for iCat CT Scanner, and all Materialise Dental software.

ACCOUNT EXECUTIVE, TAXBACK INTERNATIONAL, DUBLIN, IRELAND — 2002

Company traditionally assisted in income tax returns for holiday makers. Responsibility was for development of company diversification into Value Added Tax (V.A.T.) returns for businesses that may have travelled abroad for trading purposes.

Developed and implemented information gathering methodology.

Liaised daily with clients with respect to building relationship and maximise V.A.T. refunds from business travel.

SKILLS / AWARDS

IRCSET Scholarship 2005 (Irish Research Council for Science Education and Technology). First awardee in Physics in the DIT to receive this prestigious award.

FOCAS Award for academic achievement, 2004.

LIS Award for academic achievement, 2001/2.

Working knowledge of Fortran 77 & 90/95, C, C++, HTML and computer architecture.

Basic knowledge of Java.

Hobby roboticist.

Member of the Institute of Physics(AMinstP).

Student member of the American Physical Society.

Basic First Aid certificate, served for 3 years as a volunteer first-aider with the Tallaght Unit of the Order of Malta Ambulance Corps.

Served in the Irish Reserve Army for 3 years, achieved rank of 3* Private.

PUBLICATIONS

Currently finalising two papers: The 3C(111) and 6H(0001) SiC Mott-Hubbard Transition, Potassium Overlayers on the SiC(100) surface.

American Physical Society, March Meeting, New Orleans, March 2008, talk, "Computational Atomic Structure of the Si(111)-4x1-In System"

Condensed Matter and Materials Physics(CMMP) Conference.,April 2007, talk, "RAS Calculation of Metallic Overlayers on Silicon"

I.O.P Spring Weekend, poster "Computational results of the In-Si(111) Surface", 2006.

REFERRALS

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