

# BARRY HAYCOCK

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**PROFILE** Computational Solid State Physicist. Currently employed in the Lewis Group in West Virginia University. An IRCSET Scholar.

**EXPERIENCE** **POSTDOC RESEARCH ASSISTANT**  
*West Virginia University, WV 26501* *2011-Present*

**PH.D. STUDENT**  
*Dublin Institute of Technology, Dublin, Ireland* *2004-2011*

**EDUCATION** **DUBLIN INSTITUTE OF TECHNOLOGY**  
*Dublin, Ireland — Ph.D. Physics, Successfully defended June 10<sup>th</sup> 2011*  
Thesis “**Calculation of Electronic and Optical Properties of Nanoscale Systems**” - Development of computational codes, application to computational modeling of real world systems, determination of electronic structure of silicon carbide and silicon surfaces with metallic overlayers.  
Available at [www.barryhaycock.com](http://www.barryhaycock.com)

**DUBLIN INSTITUTE OF TECHNOLOGY**  
*Dublin Ireland — B.Sc. Physics & Physics Technology, 2004*

**INSTITUTE OF TECHNOLOGY, TALLAGHT**  
*Dublin, Ireland — Higher Diploma, Physics & Instrumentations, 2002*

**INSTITUTE OF TECHNOLOGY, TALLAGHT**  
*Dublin, Ireland — Higher Certificate, Physics & Instrumentations, 2001*

**CURRENT COLLABORATIONS** José Ortega (Universidad Autonoma de Madrid), Pavel Jelinek and Prokop Hapala (Czech Academy of Sciences), Talat Rahman, (UC Florida) developments to local-orbital density-functional based electronic-structure code (**FIREBALL**).

Christopher Matranga (NIST, Pittsburgh), Delafoissite Materials.

Karl Johnson (University of Pittsburgh), Metal Oxide Frameworks.

**PUBLICATIONS** **B. Haycock**, M.K. Underwood, and J.P. Lewis, “High-Throughput Calculations of Alloyed Delafoissite Materials: Application to  $\text{CuGa}_{1-x}\text{Fe}_x\text{O}_2$ ”, (2013 Submitted *J. Comp. Phys.*)

J. Lekse, **B. Haycock**, J. P. Lewis & C. Matranga, “The Effect of Electronic Structure Changes in  $\text{NaInO}_2$  and  $\text{NaIn}_{0.9}\text{Fe}_{0.1}\text{O}_2$  on the Photoreduction of Methylene Blue”, in preparation, 2013

**B. Haycock**, D. G. Trabada, J. Ortega, J.D. O’Mahony, and J.P. Lewis, “Metalization of the K-overlayer on the  $\beta\text{-SiC}(100) c(4\times 2)$  Surface,” *J. Phys.: Condens. Matter* 24 (2012) 485001

**B. Haycock**, D. G. Trabada, J. Ortega, J.D. O’Mahony, and J.P. Lewis, “Soft phonon effects on the electronic structure of the silicon-poor 3C-SiC(111) and 6H-SiC(0001) surfaces,” *Phys. Rev. Lett.* (In revision)

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M.K. Underwood, **B. Haycock**, J. Lekse, C. Matranga, and J. P. Lewis<sup>†,\*</sup>  
“Strain-Induced Photoabsorption in Transparent Conducting Oxide  
CuGa<sub>1-x</sub>FexO<sub>2</sub> Delafossites” 2013 (*In preparation*)

**B. Haycock**, J. Ortega, and Lewis, J. P. (2011), “Failure of potassium dimer  
formation on the  $\beta$ -SiC(100)-c(4 × 2) surface.” *physica status solidi (b)*,  
**248**: 2072–2075. doi: 10.1002/pssb.201147170

Lewis, J. P., Jelínek, P., Ortega, J., Demkov, A. A., Trabada, D. G., **Haycock, B.**,  
Wang, H., Adams, G., Tomfohr, J. K., Abad, E., Wang, H. and Drabold, D. A.  
(2011), “Advances and applications in the FIREBALL *ab initio* tight-binding  
molecular-dynamics formalism.” *physica status solidi (b)*, **248**: 1989–2007.  
doi: 10.1002/pssb.201147259

## PRESENTATIONS

American Physical Society, March Meeting, Baltimore, March 2013,  
presentation, “High-Throughput Investigation of Delafossite materials”

Hosted “FIREBALL World Congress” for developers of *ab-initio* MD code in the  
University of Central Florida, Orlando, June 18th -21st 2012. Chaired all scientific  
sessions and planning meeting, delivered 10 hours of technical lectures (2  
sessions per day).

WVU High Performance Computing Summer Institute, talk “Introduction to  
the FIREBALL *ab-initio* MD package” 2012 and 2013

American Physical Society, March Meeting, Dallas, March 2011,  
talk, “K-Induced Semiconducting to Metallic Transition on the  $\beta$ -SiC(100)  
c(4x2) 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, Birr Castle, Ireland, March 2006  
poster “Computational results of the In-Si(111) Surface”

## SKILLS / AWARDS

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

FOCAS Award for academic achievement, 2004.

LIS Award for academic achievement, 2001/2002.

## OTHER INFORMATION

XSede Computing Campus Champion, WVU.

Active mentor of the high school robotics team “MARS”.

Services include: Peer review of papers for *Physica Status Solidi* and *The Journal  
of Physical Chemistry*.

Coordinator of the FIREBALL package development.

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### REFERRALS

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Chemistry and Surface Science Division  
National Energy Technology Laboratory  
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