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Research output

Structural and Electronic Reconstruction of Extended Defects in Pnictogen Chalcogenides

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First-principles calculations of defects near a grain boundary in MgO

McKenna, K. P. & Shluger, A. L., 25 Jun 2009, In: *Physical Review B*. 79, 22, 11 p., 224116.

Gold nanoparticles under gas pressure

McKenna, K. P., 2009, In: *Physical Chemistry Chemical Physics*. 11, 21, p. 4145-4151 7 p.

Tuning Photoluminescence Properties of Alkaline-earth Oxide Nanoparticles by Site-selective Functionalization and Doping

Sushko, P. V., McKenna, K. P., Shluger, A. L. & Diwald, O., 2009, In: ECS Transactions. 25, 9, p. 131-139 9 p.

Unique bonding in nanomaterials and powders

McKenna, K. P., 2009, *Nanoscale Materials in Chemistry*. Klabunde, K. & Richards, R. (eds.). 2nd Edition ed. Wiley-Blackwell, p. 15-36 22 p.

Electron-trapping polycrystalline materials with negative electron affinity

McKenna, K. P. & Shluger, A. L., Nov 2008, In: Nature Materials. 7, 11, p. 859-862 4 p.

Origin of the asymmetry in the magnitude of the statistical variability of n- and p-channel poly-Si gate bulk MOSFETs

Asenov, A., Cathignol, A., Cheng, B., McKenna, K. P., Brown, A. R., Shluger, A. L., Chanemougame, D., Rochereau, K. & Ghibaudo, G., Aug 2008, In: IEEE Electron Device Letters. 29, 8, p. 913-915 3 p.

Shaping the morphology of gold nanoparticles by CO adsorption

McKenna, K. P. & Shluger, A. L., 27 Dec 2007, In: Journal of Physical Chemistry C. 111, 51, p. 18848-18852 5 p.

Quantum simulations of spin-relaxation and transport in copper

McKenna, K. P. & Morgan, G. J., Oct 2007, In: European physical journal b. 59, 4, p. 451-456 6 p.

Inside powders: A theoretical model of interfaces between MgO nanocrystallites

McKenna, K. P., Sushko, P. V. & Shluger, A. L., 11 Jul 2007, In: Journal of the American Chemical Society. 129, 27, p. 8600-8608 9 p.

Dynamics of low-coordinated surface atoms on gold nanocrystallites

McKenna, K. P., Sushko, P. V. & Shluger, A. L., 21 Apr 2007, In: Journal of Chemical Physics. 126, 15, 9 p., 154704.

Transient atomic configurations of supported gold nanocrystallites at finite temperature

McKenna, K. P., Sushko, P. V. & Shluger, A. L., 22 Feb 2007, In: Journal of Physical Chemistry C. 111, 7, p. 2823-2826 4 p.

Quantum transport simulation based on an equation of motion method: an application to current-perpendicular-to-the-plane giant magnetoresistance

McKenna, K. P., Michez, L. A., Morgan, G. J. & Hickey, B. J., Aug 2005, In: Physical Review B. 72, 5, p. - 7 p., 054418.

The simulation of the electronic transport properties of nanoscale devices

McKenna, K. P., 2005, University of Leeds;. 180 p.

Activities

PhD examination at Royal Holloway University of London

McKenna, K. P. (Examiner (external))

24 Aug 2021

NECEM Workshop on Interfaces in Thin-Film Photovoltaics

McKenna, K. P. (Organiser)

29 Mar 2021 → 30 Mar 2021

Psi-k working group C2: Functional materials and device (Event)

McKenna, K. P. (Chair)

2021 → ...

Density Functional Theory Simulations

McKenna, K. P. (Invited speaker)

3 Sept 2020

PhD examination at Imperial College London

McKenna, K. P. (Examiner (external))

12 Sept 2019

Charge carrier trapping in nanocrystalline anatase TiO₂

McKenna, K. P. (Speaker)

26 Jul 2019

Advanced Materials Show

McKenna, K. P. (Organiser)

10 Jul 2019 → 11 Jul 2019

Understanding the Role of Extended Defects in Resistive Switching and Magnetic Memory Materials

McKenna, K. P. (Invited speaker)

28 Jun 2019

Structure and properties of extended defects in spintronic materials through first principles calculations and electron microscopy

McKenna, K. P. (Invited speaker)

12 Jun 2019

Structure and properties of extended defects in materials through first principles calculations and electron microscopy

McKenna, K. P. (Chair)

12 Mar 2019

First principles modelling of grain boundaries in (FA/Cs)Pb(I/Br)₃ perovskite solar absorbers

McKenna, K. P. (Speaker)

12 Feb 2019

First principles modelling of grain boundaries in (FA/Cs)Pb(I/Br)₃ perovskite solar absorbers

McKenna, K. P. (Speaker)

28 Nov 2018

YorNight 2018

McKenna, K. P. (Organiser), El-Masmane, A. R. (Curator), Quirk, J. A. (Curator) & Tong, C. (Curator)

17 Nov 2018

Structure and properties of extended defects in materials through first principles calculations and electron microscopy

McKenna, K. P. (Invited speaker)

7 Nov 2018

UK High End Computing Materials Chemistry Consortium (UK HEC MCC) (External organisation)

McKenna, K. P. (Member)

Oct 2018 → ...

Modelling Electron Trapping in Titanium Dioxide

McKenna, K. P. (Speaker)

5 Mar 2018 → 9 Mar 2018

Cogent Power

McKenna, K. P. (Visitor), Thompson, S. M. (Visitor) & Pratt, A. (Visitor)
8 Feb 2018 → 9 Feb 2018

PhD examination at Imperial College London

McKenna, K. P. (Examiner (external))
19 Jan 2018

Psi-k working group C2: Functional materials and device (Event)

McKenna, K. P. (Member)
2018 → ...

The role of metal-oxide grain boundaries for applications in photovoltaics and spintronics

McKenna, K. P. (Invited speaker)
29 Nov 2017

Invited talk: The role of metal-oxide grain boundaries for applications in photovoltaics and spintronics

McKenna, K. P. (Invited speaker)
10 Jul 2017 → 12 Jul 2017

Psi-k workshop: Atomic scale materials microscopy: theory meets experiment

McKenna, K. P. (Organiser)
26 Jun 2017 → 28 Jun 2017

Invited talk: "Understanding defects in metal oxide materials"

McKenna, K. P. (Invited speaker)
22 Jun 2017

Invited talk at Institute of Engineering Innovation, School of Engineering, The University of Tokyo

McKenna, K. P. (Invited speaker)
6 Jun 2017

Invited talk in group of Prof Ulrike Diebold

McKenna, K. P. (Invited speaker)
23 Apr 2017 → 25 Apr 2017

Launch of Centre for Energy Efficient Materials

McKenna, K. P. (Organiser)
28 Mar 2017

York Centre for Energy Efficient Materials / KTN Meeting

McKenna, K. P. (Host)
5 Jan 2017

PhD examination at Aalto University

McKenna, K. P. (Examiner (external))
15 Oct 2016

Invited talk: Understanding Defects in Metal Oxide Materials

McKenna, K. P. (Invited speaker)
14 Oct 2016

Workshop on Charge Trapping Defects in Semiconductors and Insulators

McKenna, K. P. (Organiser)

1 Oct 2016 → 31 Mar 2017

Conference of the Society of Physicists of Macedonia 2016

McKenna, K. P. (Invited speaker)

24 Sept 2016

Atomic structure of nanosystems from first-principles simulations and microscopy experiments (AS-SIMEX 2016)

McKenna, K. P. (Invited speaker)

31 May 2016

Electron trapping in nanocrystalline titanium dioxide

McKenna, K. P. (Invited speaker)

20 Apr 2016

MRS Spring Meeting 2016

McKenna, K. P. (Speaker)

30 Mar 2016

MRS Spring Meeting 2016

McKenna, K. P. (Speaker)

30 Mar 2016

MRS Spring Meeting 2016

McKenna, K. P. (Speaker)

30 Mar 2016

INSTITUTE OF PHYSICS (IOP) (External organisation)

McKenna, K. P. (Member)

23 Feb 2016

Extended defects in oxides

McKenna, K. P. (Invited speaker)

28 Jan 2016

N8 HPC meeting

McKenna, K. P. (Participant)

21 Jan 2016

N8 HPC Network Event - New approaches to atomistic / quantum simulation of materials

McKenna, K. P. (Participant)

8 Jan 2016

COST Action CM1104 "Reducible Oxide Chemistry, Structure and Functions" 2015 Annual Meeting of the Working Group 4 "Reducible Oxides"

McKenna, K. P. (Invited speaker)

23 Oct 2015

Psi-k 2015 Conference

McKenna, K. P. (Participant)

6 Sept 2015 → 10 Sept 2015

19th Conference on "Insulating Films on Semiconductors

McKenna, K. P. (Participant)

30 Jun 2015 → 2 Jul 2015

Developments in Teaching Physics Students' Computer Programming Skills

McKenna, K. P. (Participant)

2 Jun 2015

National Institute for Materials Science

McKenna, K. P. (Collaborator)

9 Apr 2015 → 11 Apr 2015

Understanding defects in metal-oxide materials

McKenna, K. P. (Invited speaker)

9 Apr 2015

WPI AIMR, Tohoku University, Sendai

McKenna, K. P. (Collaborator)

5 Apr 2015 → 9 Apr 2015

University of Salzburg

McKenna, K. P. (Visitor)

14 Mar 2015 → 21 Mar 2015

Towards Reality in Nanoscale Materials VIII

McKenna, K. P. (Speaker)

9 Feb 2015 → 11 Feb 2015

HPC for Quantum Materials Simulation

McKenna, K. P. (Participant)

9 Jan 2015

Materials Chemistry Consortium Meeting

McKenna, K. P. (Participant)

6 Nov 2014

Second International Conference of Young Researchers on Advanced Materials

McKenna, K. P. (Organiser)

24 Oct 2014 → 29 Oct 2014

Gordon Research Conference: Defects in Semiconductors - Power, Efficiency, and Functionality

McKenna, K. P. (Invited speaker)

3 Aug 2014 → 8 Aug 2014

PhD examination at Nottingham Trent University

McKenna, K. P. (Examiner (external))

25 Jul 2014

International CECAM-Workshop "Nanostructured Zinc Oxide and related materials"

McKenna, K. P. (Invited speaker)

23 Jun 2014 → 27 Jun 2014

Thin Film Oxide Coatings: recent developments and applications

McKenna, K. P. (Participant)

16 Apr 2014

COST CM1104 - WG4 meeting

McKenna, K. P. (Invited speaker)

10 Apr 2014 → 11 Apr 2014

Materials Chemistry Consortium Meeting

McKenna, K. P. (Participant)

4 Apr 2014

EPSRC Early Career Researchers Retreat

McKenna, K. P. (Invited speaker)

5 Mar 2014 → 6 Mar 2014

Structure and Electronic Properties of Polycrystalline Dielectrics

McKenna, K. P. (Invited speaker)

26 Feb 2014

PhD examination at Department of Applied Physics in Aalto University

McKenna, K. P. (Examiner (external))

24 Jan 2014

Invited talk at Department of Applied Physics in Aalto University

McKenna, K. P. (Invited speaker)

23 Jan 2014

Materials Chemistry Consortium Meeting

McKenna, K. P. (Participant)

5 Nov 2013

PhD examination at Cambridge University Electrical Engineering Department

McKenna, K. P. (Examiner (external))

29 Oct 2013

Functional oxides for emerging technologies

McKenna, K. P. (Invited speaker)

14 Oct 2013 → 18 Oct 2013

National Institute for Materials Science

McKenna, K. P. (Collaborator)

23 Sept 2013 → 26 Sept 2013

WPI AIMR, Tohoku University, Sendai

McKenna, K. P. (Collaborator)

14 Sept 2013 → 20 Sept 2013

4th International Conference on Semiconductor Technology for Ultra Large Scale Integrated Circuits and Thin Film Transistors

McKenna, K. P. (Invited speaker)

7 Jul 2013 → 12 Jul 2013

Invited seminar at Institute of Electronic Materials at the Peter Grünberg Institute, Jülich

McKenna, K. P. (Invited speaker)

3 Jul 2013

COST CM1104 - WG4 meeting

McKenna, K. P. (Invited speaker)

9 May 2013 → 10 May 2013

Materials Chemistry Consortium Meeting

McKenna, K. P. (Participant)

3 May 2013

Towards Reality in Nanoscale Materials VI

McKenna, K. P. (Invited speaker)

11 Feb 2013 → 13 Feb 2013

Materials Chemistry Consortium Meeting

McKenna, K. P. (Participant)

5 Nov 2012

PhD Examination at Nanyang Technological University

McKenna, K. P. (Examiner (external))

31 Oct 2012

CMD-24

McKenna, K. P. (Invited speaker)

3 Sept 2012 → 7 Sept 2012

Materials Chemistry Consortium Meeting

McKenna, K. P. (Participant)

16 Jul 2012

2nd TYC Energy Materials Workshop

McKenna, K. P. (Speaker)

6 Jun 2012 → 8 Jun 2012

Computational Oxide Spintronics

McKenna, K. P. (Participant)

7 May 2012 → 10 May 2012

Materials Chemistry Consortium Meeting

McKenna, K. P. (Participant)

28 Mar 2012

Condensed Matter and Materials Physics 2011

McKenna, K. P. (Speaker)

13 Dec 2011 → 15 Dec 2011

Materials Chemistry Consortium Meeting

McKenna, K. P. (Invited speaker)

4 Oct 2011

Tohoku Univ, WPI AIMR, Aoba Ku

McKenna, K. P. (Researcher)

5 Sept 2011 → ...

Projects

Assessing the environmental impacts of engineered nanoparticles

MCKENNA, K. P. (Co-investigator), YUAN, J. (Principal investigator), TEAR, S. (Co-investigator) & Boxall, A. B. A. (Co-investigator)

14/03/12 → 31/07/12

Atomistic understanding of extended defects in reduced tungsten oxide to guide the optimisation of properties for energy applications

MCKENNA, K. P. (Principal investigator)

EPSRC

1/02/25 → 31/01/28

Award of computational time on the national supercomputer

McKenna, K. P. (Principal investigator)

1/11/11 → 31/01/16

Crack-tolerant materials for next-generation photovoltaics

McKenna, K. P. (Principal investigator), Dhimish, M. (Co-investigator) & LYNCH, T. (Student)

2/10/23 → 1/01/27

EPSRC IAA 2017: Centre for Energy Efficient Materials (CEEM)

MCKENNA, K. P. (Principal investigator)

EPSRC

1/01/18 → 31/12/19

EPSRC IAA joint funding for centre (McKenna)

MCKENNA, K. P. (Principal investigator)

EPSRC

1/10/16 → 30/10/17

EPSRC IAA: Next-Generation Vertically Mounted Bifacial Solar Panels: Conceptualisation, Field Testing, and Energy Performance Monitoring

Dhimish, M. (Principal investigator), McKenna, K. P. (Co-investigator) & Badran, G. (Researcher)

2/01/23 → 31/05/24

First principles investigation of polaron mobility in nanocrystalline titanium dioxide

McKenna, K. P. (Principal investigator)

1/07/13 → 30/08/13

Half-metallic Ferromagnets: materials fundamentals for next-generation spintronics

LAZAROV, V. (Principal investigator), HIROHATA, A. (Co-investigator) & MCKENNA, K. P. (Co-investigator)

EPSRC

1/10/13 → 31/01/18

High-throughput screening of polycrystalline solar absorbers (Ext.)

MCKENNA, K. P. (Principal investigator)

EPSRC

1/01/18 → 31/03/21

International Network for Spintronics: From Material development to Novel Energy Efficient Technologies

MCKENNA, K. P. (Principal investigator) & HIROHATA, A. (Co-investigator)

EPSRC

1/04/21 → 30/04/28

Non-equilibrium electron-ion dynamics in thin metal-oxide

MCKENNA, K. P. (Principal investigator)

EPSRC
1/01/13 → 30/04/18

Optimisation of charge carrier mobility in nanoporous metal oxide films

MCKENNA, K. P. (Principal investigator), CHECHIK, V. (Co-investigator), DOUTHWAITE, R. E. (Co-investigator) & LAZAROV, V. (Co-investigator)

EPSRC
1/01/17 → 31/10/20

PhOCUS: Photonic optimisation of catalysis under sunlight

Douthwaite, R. E. (Principal investigator), McKenna, K. P. (Co-investigator), COCKETT, M. C. R. (Co-investigator), Parkin, A. (Co-investigator) & Krauss, T. F. (Co-investigator)

1/02/14 → 30/06/14

Plasma assisted CO₂ catalysis

McKenna, K. P. (Co-investigator) & NORTH, M. (Principal investigator)

19/04/13 → 31/07/13

QUANTum Transport for Advanced Spintronics

CAVILL, S. A. (Principal investigator), AVESTRO, A.-J. (Co-investigator), DOUTHWAITE, R. E. (Co-investigator), EVANS, R. F. L. (Co-investigator), Ferreira, A. F. (Co-investigator), LAZAROV, V. (Co-investigator), MCKENNA, K. P. (Co-investigator), PRATT, A. (Co-investigator), VALLEJO FERNANDEZ, G. (Co-investigator) & XU, Y. (Co-investigator)

EPSRC
1/10/22 → 30/09/25

RPF 13/14 High-energy-resolution spectroscopy of functional nanomaterials

McKenna, K. P. (Co-investigator), Lazarov, V. (Principal investigator), Clark, J. H. (Co-investigator) & Pratt, A. (Co-investigator)

1/08/13 → 31/07/14

RPF 2015/16 Solar energy conversion: Measurement of efficiency as a function of wavelength

Douthwaite, R. E. (Principal investigator) & McKenna, K. P. (Co-investigator)

1/08/15 → 31/07/16

Tailoring structure–property relationships in metal halide perovskites at an atomistic level

MCKENNA, K. P. (Principal investigator)

EPSRC
1/03/26 → 31/08/29

UKRI CoA Extension to R1788002 Optimisation of charge carrier mobility in nanoporous metal oxide films

DOUTHWAITE, R. E. (Principal investigator), CHECHIK, V. (Co-investigator), LAZAROV, V. (Co-investigator) & MCKENNA, K. P. (Co-investigator)

EPSRC
1/11/20 → 28/02/21

UKRI CoA Extension to R1845501 High-throughput screening of polycrystalline solar absorbers

MCKENNA, K. P. (Principal investigator)

EPSRC
1/04/21 → 30/06/21