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## Research output

### Grain-Boundary Structural Relaxation in $\text{Sb}_2\text{Se}_3$ Thin-Film Photovoltaics

Lomas-Zapata, R. A., McKenna, K. P., Ramasse, Q. M., Williams, R. E., Phillips, L. J., Durose, K., Major, J. D. & Mendis, B. G., 8 Feb 2024, In: PRX Energy. 3, 1, 10 p., 013006.

### Grain boundaries in polycrystalline materials for energy applications: First principles modeling and electron microscopy

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### Cu-Zn Cation Disorder in Kesterite $\text{Cu}_2\text{ZnSn}(\text{SxSe}_{1-x})_4$ Solar Cells

Zhu, A-Y., Ding, R-X., Xu, H-T., Tong, C-J. & McKenna, K. P., 19 Jan 2024, In: ACS Energy Letters. 9, p. 497-503 7 p.

### Thermodynamic properties and switching dynamics of perpendicular shape anisotropy MRAM

Lack, W., Jenkins, S., Meo, A., Chantrell, R. W., McKenna, K. P. & Evans, R. F. L., 5 Jan 2024, In: Journal of Physics Condensed Matter. 36, 14, 15 p., 145801.

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Elser, M. J., Neige, E., Berger, T., Chiesa, M., Giamello, E., McKenna, K., Risse, T. & Diwald, O., 11 May 2023, In: Journal of Physical Chemistry C. 127, 18, p. 8778-8787 10 p.

### Small-polaron mediated recombination in titanium dioxide from first principles

Quirk, J. A. & McKenna, K. P., 1 May 2023, In: Physical Review Research. 5, 2, 8 p., 023072.

### Heterogeneity of grain boundary properties in $\text{Cu}_2\text{ZnSnS}_4$ : A first-principles study

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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**

Keith Patrick McKenna (Examiner (external))

24 Aug 2021

**NECEM Workshop on Interfaces in Thin-Film Photovoltaics**

Keith Patrick McKenna (Organiser)

29 Mar 2021 → 30 Mar 2021

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

Keith Patrick McKenna (Chair)

2021 → ...

**Density Functional Theory Simulations**

Keith Patrick McKenna (Invited speaker)

3 Sept 2020

**PhD examination at Imperial College London**

Keith Patrick McKenna (Examiner (external))

12 Sept 2019

**Charge carrier trapping in nanocrystalline anatase TiO<sub>2</sub>**

Keith Patrick McKenna (Speaker)

26 Jul 2019

**Advanced Materials Show**

Keith Patrick McKenna (Organiser)



10 Jul 2019 → 11 Jul 2019

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

Keith Patrick McKenna (Invited speaker)

28 Jun 2019

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

Keith Patrick McKenna (Invited speaker)

12 Jun 2019

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

Keith Patrick McKenna (Chair)

12 Mar 2019

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

Keith Patrick McKenna (Speaker)

12 Feb 2019

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

Keith Patrick McKenna (Speaker)

28 Nov 2018

**YorNight 2018**

Keith Patrick McKenna (Organiser), Abdul Razak El-Maslmene (Curator), James Anthony Quirk (Curator) & Chuanjia Tong (Curator)

17 Nov 2018

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

Keith Patrick McKenna (Invited speaker)

7 Nov 2018

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

Keith Patrick McKenna (Member)

Oct 2018 → ...

**Modelling Electron Trapping in Titanium Dioxide**

Keith Patrick McKenna (Speaker)

5 Mar 2018 → 9 Mar 2018

**Cogent Power**

Keith Patrick McKenna (Visitor), Sarah Madeleine Thompson (Visitor) & Andrew Pratt (Visitor)

8 Feb 2018 → 9 Feb 2018

**PhD examination at Imperial College London**

Keith Patrick McKenna (Examiner (external))

19 Jan 2018

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

Keith Patrick McKenna (Member)

2018 → ...

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

Keith Patrick McKenna (Invited speaker)

29 Nov 2017

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

Keith Patrick McKenna (Invited speaker)

10 Jul 2017 → 12 Jul 2017

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

Keith Patrick McKenna (Organiser)

26 Jun 2017 → 28 Jun 2017

**Invited talk: "Understanding defects in metal oxide materials"**

Keith Patrick McKenna (Invited speaker)

22 Jun 2017

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

Keith Patrick McKenna (Invited speaker)

6 Jun 2017

**Invited talk in group of Prof Ulrike Diebold**

Keith Patrick McKenna (Invited speaker)

23 Apr 2017 → 25 Apr 2017

**Launch of Centre for Energy Efficient Materials**

Keith Patrick McKenna (Organiser)

28 Mar 2017

**York Centre for Energy Efficient Materials / KTN Meeting**

Keith Patrick McKenna (Host)

5 Jan 2017

**PhD examination at Aalto University**

Keith Patrick McKenna (Examiner (external))

15 Oct 2016

**Invited talk: Understanding Defects in Metal Oxide Materials**

Keith Patrick McKenna (Invited speaker)

14 Oct 2016

**Workshop on Charge Trapping Defects in Semiconductors and Insulators**

Keith Patrick McKenna (Organiser)

1 Oct 2016 → 31 Mar 2017

**Conference of the Society of Physicists of Macedonia 2016**

Keith Patrick McKenna (Invited speaker)

24 Sept 2016

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

Keith Patrick McKenna (Invited speaker)

31 May 2016

**Electron trapping in nanocrystalline titanium dioxide**

Keith Patrick McKenna (Invited speaker)

20 Apr 2016

**MRS Spring Meeting 2016**  
Keith Patrick McKenna (Speaker)  
30 Mar 2016

**MRS Spring Meeting 2016**  
Keith Patrick McKenna (Speaker)  
30 Mar 2016

**MRS Spring Meeting 2016**  
Keith Patrick McKenna (Speaker)  
30 Mar 2016

**INSTITUTE OF PHYSICS (IOP) (External organisation)**  
Keith Patrick McKenna (Member)  
23 Feb 2016

**Extended defects in oxides**  
Keith Patrick McKenna (Invited speaker)  
28 Jan 2016

**N8 HPC meeting**  
Keith Patrick McKenna (Participant)  
21 Jan 2016

**N8 HPC Network Event - New approaches to atomistic / quantum simulation of materials**  
Keith Patrick McKenna (Participant)  
8 Jan 2016

**COST Action CM1104 "Reducible Oxide Chemistry, Structure and Functions" 2015 Annual Meeting of the Working Group 4 "Reducible Oxides"**  
Keith Patrick McKenna (Invited speaker)  
23 Oct 2015

**Psi-k 2015 Conference**  
Keith Patrick McKenna (Participant)  
6 Sept 2015 → 10 Sept 2015

**19th Conference on "Insulating Films on Semiconductors"**  
Keith Patrick McKenna (Participant)  
30 Jun 2015 → 2 Jul 2015

**Developments in Teaching Physics Students' Computer Programming Skills**  
Keith Patrick McKenna (Participant)  
2 Jun 2015

**National Institute for Materials Science**  
Keith Patrick McKenna (Collaborator)  
9 Apr 2015 → 11 Apr 2015

**Understanding defects in metal-oxide materials**  
Keith Patrick McKenna (Invited speaker)  
9 Apr 2015

**WPI AIMR, Tohoku University, Sendai**  
Keith Patrick McKenna (Collaborator)

5 Apr 2015 → 9 Apr 2015

**University of Salzburg**

Keith Patrick McKenna (Visitor)

14 Mar 2015 → 21 Mar 2015

**Towards Reality in Nanoscale Materials VIII**

Keith Patrick McKenna (Speaker)

9 Feb 2015 → 11 Feb 2015

**HPC for Quantum Materials Simulation**

Keith Patrick McKenna (Participant)

9 Jan 2015

**Materials Chemistry Consortium Meeting**

Keith Patrick McKenna (Participant)

6 Nov 2014

**Second International Conference of Young Researchers on Advanced Materials**

Keith Patrick McKenna (Organiser)

24 Oct 2014 → 29 Oct 2014

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

Keith Patrick McKenna (Invited speaker)

3 Aug 2014 → 8 Aug 2014

**PhD examination at Nottingham Trent University**

Keith Patrick McKenna (Examiner (external))

25 Jul 2014

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

Keith Patrick McKenna (Invited speaker)

23 Jun 2014 → 27 Jun 2014

**Thin Film Oxide Coatings: recent developments and applications**

Keith Patrick McKenna (Participant)

16 Apr 2014

**COST CM1104 - WG4 meeting**

Keith Patrick McKenna (Invited speaker)

10 Apr 2014 → 11 Apr 2014

**Materials Chemistry Consortium Meeting**

Keith Patrick McKenna (Participant)

4 Apr 2014

**EPSRC Early Career Researchers Retreat**

Keith Patrick McKenna (Invited speaker)

5 Mar 2014 → 6 Mar 2014

**Structure and Electronic Properties of Polycrystalline Dielectrics**

Keith Patrick McKenna (Invited speaker)

26 Feb 2014

**PhD examination at Department of Applied Physics in Aalto University**

Keith Patrick McKenna (Examiner (external))

24 Jan 2014

**Invited talk at Department of Applied Physics in Aalto University**

Keith Patrick McKenna (Invited speaker)

23 Jan 2014

**Materials Chemistry Consortium Meeting**

Keith Patrick McKenna (Participant)

5 Nov 2013

**PhD examination at Cambridge University Electrical Engineering Department**

Keith Patrick McKenna (Examiner (external))

29 Oct 2013

**Functional oxides for emerging technologies**

Keith Patrick McKenna (Invited speaker)

14 Oct 2013 → 18 Oct 2013

**National Institute for Materials Science**

Keith Patrick McKenna (Collaborator)

23 Sept 2013 → 26 Sept 2013

**WPI AIMR, Tohoku University, Sendai**

Keith Patrick McKenna (Collaborator)

14 Sept 2013 → 20 Sept 2013

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

Keith Patrick McKenna (Invited speaker)

7 Jul 2013 → 12 Jul 2013

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

Keith Patrick McKenna (Invited speaker)

3 Jul 2013

**COST CM1104 - WG4 meeting**

Keith Patrick McKenna (Invited speaker)

9 May 2013 → 10 May 2013

**Materials Chemistry Consortium Meeting**

Keith Patrick McKenna (Participant)

3 May 2013

**Towards Reality in Nanoscale Materials VI**

Keith Patrick McKenna (Invited speaker)

11 Feb 2013 → 13 Feb 2013

**Materials Chemistry Consortium Meeting**

Keith Patrick McKenna (Participant)

5 Nov 2012

**PhD Examination at Nanyang Technological University**

Keith Patrick McKenna (Examiner (external))

31 Oct 2012

**CMD-24**

Keith Patrick McKenna (Invited speaker)

3 Sept 2012 → 7 Sept 2012

**Materials Chemistry Consortium Meeting**

Keith Patrick McKenna (Participant)

16 Jul 2012

**2nd TYC Energy Materials Workshop**

Keith Patrick McKenna (Speaker)

6 Jun 2012 → 8 Jun 2012

**Computational Oxide Spintronics**

Keith Patrick McKenna (Participant)

7 May 2012 → 10 May 2012

**Materials Chemistry Consortium Meeting**

Keith Patrick McKenna (Participant)

28 Mar 2012

**Condensed Matter and Materials Physics 2011**

Keith Patrick McKenna (Speaker)

13 Dec 2011 → 15 Dec 2011

**Materials Chemistry Consortium Meeting**

Keith Patrick McKenna (Invited speaker)

4 Oct 2011

**Tohoku Univ, WPI AIMR, Aoba Ku**

Keith Patrick McKenna (Researcher)

5 Sept 2011 → ...

**Projects****Assessing the environmental impacts of engineered nanoparticles**

McKenna, K. P., Yuan, J., Tear, S. & Boxall, A. B. A.

14/03/12 → 31/07/12

**Award of computational time on the national supercomputer**

McKenna, K. P.

1/11/11 → 31/01/16

**Crack-tolerant materials for next-generation photovoltaics**

McKenna, K. P., Dhimish, M. & Lynch, T.

2/10/23 → 1/01/27

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

McKenna, K. P.

EPSRC

1/01/18 → 31/12/19

**EPSRC IAA joint funding for centre (McKenna)**

McKenna, K. P.

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., McKenna, K. P. & Badran, G.

2/01/23 → 31/05/24

**First principles investigation of polaron mobility in nanocrystalline titanium dioxide**

McKenna, K. P.

1/07/13 → 30/08/13

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

Lazarov, V., Hirohata, A. & McKenna, K. P.

EPSRC

1/10/13 → 31/01/18

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

McKenna, K. P.

EPSRC

1/01/18 → 31/03/21

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

McKenna, K. P. & Hirohata, A.

EPSRC

1/04/21 → 30/04/28

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

McKenna, K. P.

EPSRC

1/01/13 → 30/04/18

**Optimisation of charge carrier mobility in nanoporous metal oxide films**

McKenna, K. P., Chechik, V., Douthwaite, R. E. & Lazarov, V.

EPSRC

1/01/17 → 31/10/20

**PhOCUS: Photonic optimisation of catalysis under sunlight**

Douthwaite, R. E., McKenna, K. P., Cockett, M. C. R., Parkin, A. & Krauss, T. F.

1/02/14 → 30/06/14

**Plasma assisted CO<sub>2</sub> catalysis**

McKenna, K. P. & North, M.

19/04/13 → 31/07/13

**QUANTum Transport for Advanced Spintronics**

Cavill, S. A., Avestro, A., Douthwaite, R. E., Evans, R. F. L., Ferreira, A., Lazarov, V., McKenna, K. P., Pratt, A., Vallejo Fernandez, G. & Xu, Y.

EPSRC

1/10/22 → 30/09/25

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

McKenna, K. P., Lazarov, V., Clark, J. H. & Pratt, A.

1/08/13 → 31/07/14

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

Douthwaite, R. E. & McKenna, K. P.

1/08/15 → 31/07/16

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

Douthwaite, R. E., Chechik, V., Lazarov, V. & McKenna, K. P.

EPSRC

1/11/20 → 28/02/21

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

McKenna, K. P.

EPSRC

1/04/21 → 30/06/21