

# CURRICULUM VITAE

Alexander Chroneos

e-mail: [achronaios@uth.gr](mailto:achronaios@uth.gr) ; [alexander.chroneos@imperial.ac.uk](mailto:alexander.chroneos@imperial.ac.uk)

## 1 HIGHER EDUCATION

### Degrees

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|------|--|
| 2008 | PhD Defect Processes in Germanium, Department of Materials, Imperial College London.     |
| 2002 | BEng (Hons) in Civil Engineering, Department of Civil Engineering, Edinburgh University. |
| 1999 | MSc in Theoretical Chemistry, Department of Theoretical Chemistry, Oxford University.    |
| 1998 | BEng (Hons) in Materials with Physics, Department of Materials, Imperial College London. |

### Awards

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|-------------|--|
| 2016 & 2017 | Candidate of the annual ENI prize in Energy (nominated by the organization committee). |
| 1996 & 1997 | UROP scholarships, Imperial College London.  |

## 2 APPOINTMENTS AND EXPERIENCE

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|--------------|---|
| 2021-today   | Professor in Computational Modelling and Systems Simulation, Department of Electrical and Computer Engineering, University of Thessaly. |
| 2016-2021    | Professor in Materials Physics, Coventry University.  |
| 2014-2015    | Reader in Materials Physics, Coventry University.   |
| 2012-2014    | Lecturer in Energy, The Open University.  |
| 2015-present | Visiting Reader, Imperial College London.   |
| 2011-2015    | Visiting Lecturer, Imperial College London.   |
| 2011-2012    | Marie Curie Intra European Fellow, NCSR Demokritos.   |
| 2010-2011    | Research Assistant, University of Cambridge.  |

2010-2011	Visiting Academic, Imperial College London.
2010, 2013	Visiting Researcher, Massachusetts Institute of Technology.
2008-2010	Research Assistant, Imperial College London.
2008	Research Assistant, Münster University, Germany.
2003-2004	Military Service.

### 3 CONTRIBUTIONS TO TEACHING

**University of Thessaly:** Introduction to Nanoelectronics, Introduction to Computational modelling, Electrotechnical Materials

**Coventry University:** 208MAE Analytical Modelling, 2014-2015 Lectures and tutorials in mathematics and finite element modeling.

**The Open University:** TXR120/T176 Engineering: An Active Introduction, 2014 Tutor; MST124/5 Essential Mathematics, The Open University 2014 Review of module material; T894 Professional Practice Portfolio, The Open University 2013-2014 Module Team; TXR220 Engineering in Action, The Open University 2013 Tutor; T207 Engineering: Mechanics, Materials, Design, The Open University 2013 Review of module material; T884 Introduction to Finite Element Analysis, The Open University 2012 Examination and Assessment Board; T174 Engineering the Future, The Open University 2012 Proof Reading

**Imperial College Longon:** Hydrogen Production using Nuclear Energy, MSc in Nuclear Engineering, 2011-2019 Lectures, assessment, marking, Examination Board; MSE 105, BEng in Materials Science, 2008-2010 Lectures and tutorials in Atomic Theory, Waves in Solids, Quantum Theory, Crystallography and Chemical Bonding

### 4 CONTRIBUTIONS TO ADMINISTRATION AND MANAGEMENT

2014-2020	I represented Coventry University on the NAILS meeting.
2012	I was the UK lead in the European Energy Research Alliance: Joint Programme in Nuclear Materials meeting in Karlsruhe.
2012	I represented The Open University on the NAILS meeting.

### 5 RESEARCH AND SCHOLARSHIP

#### Research interests

Over 350 research papers. H-index 62 (9500+ cites). Current research interests centre in the areas of sustainable and clean energy and advanced materials. My present and future research directions include solid oxide fuel cell materials, graphene, batteries, hydrogen production, and radiation sensors. The research methods include advanced modelling techniques (for example genetic algorithms, density functional theory and molecular dynamics).

## Research funding

- 2018 Project Title: Energy HarveStorers for Powering the Internet of Things  
Funder: EU (Horizon 2020)  
Grant: 400,000 Euros
- 2018 Project Title: Studying Temperature- and Ambient-Induced Band Structure Changes in Tin Oxide  
Funder: Lloyd's Research Foundation  
Grant: 49,400 pounds  
Collaborators: Dr Maria Vasilopoulou & Dr. Dimitris Davazoglou (NCSR Demokritos)
- 2014 Project Title: LRF Centre for Nuclear Safety  
Funder: Lloyd's Research Foundation  
Grant: 500,000 pounds  
Collaborator: Prof. Mike Fitzpatrick (Coventry University)
- 2013 Project Title: Stimulate  
Funder: EU  
Grant: 96,000 Euros  
Collaborator: Dr Bernie Clark (Open University)
- 2013 Project Title: Matisse  
Funder: EU  
Grant: 22,000 Euros
- 2011 Project Title: Flexible Nuclear Power for Clean Fuels and Peak Electricity Production by Co-Electrolysis of CO<sub>2</sub> and H<sub>2</sub>O  
Funder: China (Tsingua-Cambridge-MIT Alliance)  
Grant: \$200,000  
Collaborators: Dr Paul Bristowe (Cambridge University)
- 2011 Project Title: Rare Earth Oxide Dielectrics for Advanced Ge CMOS Technology  
Funder: EU  
Grant: 154,000 Euros
- 2010 Project Title: Controlling Dopant Distribution and Structures in Advanced Semiconductors  
Funder: KAUST  
Grant: \$340,590  
Collaborator: Prof. Robin Grimes (Imperial College London)
- 2009 Project Title: Diffusion and Stability of Dopants in Ge and III-V compounds  
Funder: KAUST  
Grant: £62,936  
Collaborator: Prof. Robin Grimes (Imperial College London)
- 2005 Project Title: Simulation of Hydroxide Materials  
Funder: USAF  
Grant: \$12,000  
Collaborator: Prof. Robin Grimes (Imperial College London)

## 6 POSTGRADUATE STUDENT SUPERVISION AND EXAMINATIONS

### Postdoc supervision

- 2018-2021 Supervisor of Dr Navaratnarajah Kuganathan (Coventry University)
- 2017-2021 Supervisor of Dr Nicolaos Kelaidis (Coventry University)
- 2015-2016 Supervisor of Dr Stavros-Richard Christopoulos (Coventry University)
- 2014 Supervisor of Dr Michael Rushton (Imperial College/The Open University)

### PhD supervision

- 2020-present Co-Supervisor of Konstantina Papadopoulou (Coventry University)  
PhD Optimizing the Nanoscale Behaviour of Novel Materials for Energy Applications
- 2019-present Supervisor of Petros Filippatos (Coventry University)  
PhD Temperature and Ambient-Induced Band Structure Changes in Tin Oxide to Optimize Nanosensors for Safety Applications
- 2019-present Co-Supervisor of Sotirios Fragkos (University of West Attica)  
PhD Investigation of Topological Properties of Materials: Topological Insulators, Weyl and Dirac Semimetals
- 2016-present Co-Supervisor of Angeliki Kaiafa (University of Piraeus)  
PhD Mixed Problems of Boundary Values for Maxwell Equations
- 2015-2019 Supervisor of Olga Thoda (Coventry University)  
PhD Production and Characterization of Inorganic Cobalt-based Pigments with Combustion Synthesis
- 2015-2018 Supervisor of Apostolis Kordatos (Coventry University)  
PhD Disordered Oxides for Lithium Batteries
- 2014-2017 Co-Supervisor of Avishek Dey (The Open University)  
PhD Graphene Based Solar Cell (graduated 10/2017)
- 2010-2014 Co-Supervisor of Hassan Tahini (Imperial College London)  
PhD Modelling of Defects in Advanced Semiconductors (graduated 1/2014)

### Diploma thesis supervision

- 2017-2018 Co-Supervisor of Petros-Panagis Filippatos (National Technical University of Athens)  
Dipl. Thesis Lithium in 312 MAX Phases
- 2015 Co-Supervisor of Angeliki Kaiafa (University of Athens)  
MSc Thesis Mixed Problems of Boundary Values for Maxwell Equations (graduated 12/2015)

### **Academic visitors**

2017            Research visit (3-5/2017) by Assistant Professor Evangelia Kotta-Athanasiadou (University of Athens)

### **PhD examinations**

- 2018            External Examiner of Shahid Sattar (KAUST)  
PhD Interface Effects Enabling New Applications of Two-Dimensional Materials  
(Examined 5/2018)
- 2017            External Examiner of Salawu Omotayo Akande (KAUST) PhD First Principles Studies of Perovskites for Intermediate Temperature Solid Oxide Fuel Cell Cathodes  
(Examined 5/2017)
- 2016            External Examiner of Jiwuer Jilili (KAUST)  
PhD Manganites in Perovskite Superlattices: Structural and Electronic Properties  
(Examined 6/2016)
- 2016            External Examiner of Daniel King (University of Technology Sydney)  
PhD Investigation of High-Entropy Alloys for Use in Advanced Nuclear Applications  
(Examined 6/2016)
- 2016            External Examiner of Sergiy Grytsyuk (KAUST)  
PhD Simulation of Magnetic Phenomena at Realistic Interfaces  
(Examined 2/2016)

## **7        EXTERNAL ACADEMIC ACTIVITIES**

### **Academic editorial work**

- 2018-present   Editorial Member of Applied Science (MDPI Publishing Group).
- 2015-present   Editorial Member of Scientific Reports (Nature Publishing Group).
- 2012-present   Member of the consultative council of the Journal of Kharkov National University, "Physics" series.

### **Contribution to conferences**

- International Advisory Board, Diffusion in Materials conference (DIMAT), Münster, Germany 2014.
- Steering Committee, Workshop on Smart Energy and Power Systems (WINDASPES), Greece 2014 & 2015

### **Selected Invited lectures**

- Jun 2017        **A. Chroneos**, "*Diffusion in Energy Materials: Insights from Atomistic Modelling*," 21<sup>st</sup> International Conference on Solid State Ionics, Padova, Italy, 18-23/6/2017.

- May 2017 **A. Chroneos**, “*Modelling Materials for Energy Applications*,” 4<sup>th</sup> Erasmus week on Modern Topics in Electronics and Applications, Chania, Greece, 21-27/5/2017.
- Oct 2015 **A. Chroneos**, (keynote speaker), “*Solid State Physics Revisited*,” Smart Energy Workshop, Volos, Greece, 15-16/10/2015.
- Jul 2014 **A. Chroneos**, (keynote speaker), “*Challenges in Energy Materials*,” 5<sup>th</sup> International Conference on Information, Intelligence, Systems and Applications (IISA), Workshop on Smart Energy and Power Systems (WINDASPES), Chania, Greece, 7-9/7/2014.
- May 2014 **A. Chroneos**, “*Diffusion in Germanium*,” Dept. of Physics, National Technical University of Athens, Greece 9/5/2014.
- Jun 2013 **A. Chroneos**, “*Studies of Ionic Diffusion in Oxides for Energy Applications*,” Dept. of Nuclear Engineering, MIT, USA 18/6/2013.
- Oct 2012 **A. Chroneos**, “*Engineering Defects in Germanium*” Multiscale Materials Modeling (Symposium A: Microstructure Evolution Across Multiple Length Scales: Defects to Materials Properties), Singapore, 15-19/10/2012 (declined).
- Jul 2011 J. A. Kilner, **A. Chroneos**, D. Parfitt, I. Seymour, R. W. Grimes, and A. Tarancon, “*Intrinsic Disorder and Diffusion in LnBaCo<sub>2</sub>O<sub>5.5</sub> Double Perovskites*,” 18<sup>th</sup> International Conference on Solid State Ionics, Warsaw, Poland, 3-8/7/2011.
- May 2011 **A. Chroneos**, “*Diffusion in Materials for Microelectronic and Energy Applications*,” Dept. of Physics, National Technical University of Athens, Greece 6/5/2011.
- Apr 2011 **A. Chroneos**, “*Diffusion in Materials for Microelectronic and Energy Applications*,” Dept. of Chemical Engineering, University of Patras, Greece 8/4/2011.
- Mar 2011 **A. Chroneos**, “*Engineering Defects in Energy Materials*,” Ecole Centrale Paris, France 7/3/2011.
- Jan 2011 **A. Chroneos**, “*Advanced Materials for Energy Applications*,” Dept. of Chemical Engineering, National Technical University of Athens, Greece 31/1/2011.
- Mar 2010 **A. Chroneos**, “*Molecular Dynamics Studies of Oxygen Diffusion in Oxides for SOFC Applications*,” Dept. of Mechanical Engineering, MIT, USA 19/3/2010.
- Aug 2009 **A. Chroneos**, H. Bracht, and R. W. Grimes, “*Diffusion and Defect Reactions of Donor Atoms in Ge and SiGe*,” Thermodynamic and Transport Kinetics of Nanostructured Materials, Oranienburg, Germany 17-20/8/2009.
- Jul 2009 **A. Chroneos**, “*Dopant-Defect Interactions in Inorganic Materials*,” Institute of Transuranium Elements, Karlsruhe, Germany 10/7/2009.
- Jun 2009 H. Bracht, S. Schneider, and **A. Chroneos**, “*Technological and Scientific Aspects of Self- and Dopant Diffusion in Ge*,” European Materials Research Society Spring Meeting (Semiconductor Materials), Strasbourg, France 8-12/6/2009.

- Oct 2008      **A. Chroneos**, H. Bracht, and S. Brotzmann, "*Diffusion and Defect Reactions of Donors, Carbon, and Vacancies in Germanium*", 7<sup>th</sup> International Conference on Diffusion in Materials, Lanzarote, Spain 28-31/10/2008.
- Jun 2007      **A. Chroneos**, "*Atomistic Studies of Impurity-Vacancy Complexes in Germanium*" Institute of Materials Physics, Münster University, Münster, Germany, 4/6/2007.

## 8      OTHER INFORMATION

**Editorial Board:** Scientific Reports (Nature Publishing Group), Applied Sciences (MDPI)

**Referee in Journals:** Nature Communications, Physical Review Letters, Accounts of Chemical Research, Energy & Environmental Science, Journal of the American Chemical Society, Chemistry of Materials, ACS Applied Materials & Interfaces, Journal of Physics: Condensed Matter, Journal of Physical Chemistry Letters, Journal of Materials Chemistry A, International Materials Reviews, Journal of Power Sources, International Journal of Hydrogen Energy, Journal of Physical Chemistry, Inorganic Chemistry, Applied Physics Letters, Physical Review B, RSC Advances, Journal of the Electrochemical Society, Applied Surface Science, Journal of Physics D: Applied Physics, Chemical Physics Letters, Solid State Ionics, Applied Catalysis A, Fuel Cells, Journal of Applied Physics, Journal of Alloys and Compounds, Superconductor Science and Technology, Beilstein Journal of Nanotechnology, Materials Letters, Materials Chemistry and Physics, Solid State Communications, Journal of Solid State Electrochemistry, Computational Materials Science, European Physical Journal B, Journal of Crystal Growth, Energies, Physica Status Solidi (b), Materials Science Engineering B, Thin Solid Films, Journal of Nuclear Materials, Microelectronic Engineering, Journal of Materials Science, Philosophical Magazine, Journal of Physics and Chemistry of Solids, Physics and Chemistry of Minerals, Current Applied Physics, Physica B, IEEE Transactions on Applied Superconductivity, Materials Science and Semiconductor Processing, Materials & Design, Results in Physics, Computational Condensed Matter, Energy Storage Materials, Applied Sciences, Materials, International Journal of Modern Physics B, Nuclear Science and Techniques, Journal of Computational Methods in Sciences and Engineering, Sustainability, Acta Geophysica, Crystal Research & Technology, Indian Journal of Physics, Advances in Condensed Matter.

Referee of the Royal Society.

Referee of the Royal Academy of Engineering.

Referee of the Swiss National Science Foundation.

Referee of the Netherlands Organisation for Scientific Research.

Referee of the Austrian Science Fund.

Referee of the Georgia National Science Foundation (GNSF).

## 9      SELECTED REPRESENTATIVE PUBLICATIONS

1. F. Baiutti, F. Chiabrera, M. Acosta, D. Diercks, D. Parfitt, J. Santiso, X. Wang, A. Cavallaro, A. Morata, H. Wang, **A. Chroneos**, J. MacManus-Driscoll and A. Tarancon, "*A High-Entropy Manganite in an Ordered Nanocomposite for Long-Term Application in Solid Oxide Cells*," *Nature Commun.* **12**, 2660 (2021).

2. M. Vasilopoulou, A. B. Yusoff, N. Kuganathan, X. C. Bao, A. Verykios, E. Polydorou, K. K. Armadorou, A. Soultati, G. Papadimitropoulos, M. I. Haider, A. Fakharuddin, L. C. Palilis, S. Kennou, **A. Chroneos**, P. Argitis, and D. Davazoglou, "*A Carbon-Doped Tantalum Dioxyluoride as a Superior Electron Transport material for High Performance Organic Optoelectronics*," *Nano Energy* **70**, 104508 (2020).

3. F. Chiabrera, I. Garbayo, L. Lopez-Conesa, G. Martin, A. Ruiz-Caridad, M. Walls, L. Ruiz-Gonzalez, A. Kordatos, M. Nunez, A. Morata, S. Estrade, **A. Chroneos**, F. Peiro and A. Tarancon, “Engineering Transport in Manganites by Tuning Local Nonstoichiometry in Grain Boundaries,” *Adv. Mater.* **31**, 1805360 (2019).
4. M. Alamaniotis, J. Mathew, **A. Chroneos**, M. E. Fitzpatrick and L. H. Tsoukalas, “Probabilistic Kernel Machines for Predictive Monitoring of Weld Residual Stress in Energy Systems,” *Eng. Appl. Artif. Intel.* **71**, 138-154 (2018).
5. J. Mathew, D. Parfitt, K. Wilford, N. Riddle, M. Alamaniotis, **A. Chroneos**, and M. E. Fitzpatrick, “Reactor Pressure Vessel Embrittlement: Insights from Neural Network Modelling,” *J. Nucl. Mater.* **502**, 311-322 (2018).
6. S. Kanarachos, S. R. G. Christopoulos, **A. Chroneos**, and M. E. Fitzpatrick, “Detecting Anomalies in Time Series Data via an Algorithm Combining Wavelets, Neural Networks and Hilbert Transform,” *Expert Systems with Applications* **85**, 292-304 (2017).
7. J. Zhu, **A. Chroneos**, L. Wang, F. Rao, and U. Schwingenschlögl, “Stress-Enhanced Lithiation in MAX Compounds for Battery Applications,” *Appl. Mater. Today* **9**, 192-195 (2017).
8. J. Zhu, **A. Chroneos**, J. Eppinger, and U. Schwingenschlögl, “S-Functionalized MXenes as Electrode Materials for Li-Ion Batteries,” *Appl. Mater. Today* **5**, 19-24 (2016).
9. A. Dey, **A. Chroneos**, N. St. J. Braithwaite, R. P. Gandhiraman, and S. Krishnamurthy, “Plasma Engineering of Graphene”. *Appl. Phys. Rev.* **3**, 021301 (2016).
10. J. Zhu, **A. Chroneos**, and U. Schwingenschlögl, “Silicene/Germanene on  $MgX_2$  ( $X = Cl, Br, \text{ and } I$ ) for Li-Ion Battery Applications,” *Nanoscale* **8**, 7272-7277 (2016).
11. D. Horlait, S. C. Middleburgh, **A. Chroneos**, and W. E. Lee, “Synthesis and DFT investigation of new bismuth- containing MAX phases,” *Sci. Rep.* **6**, 18829 (2016).
12. H. A. Tahini, **A. Chroneos**, S. C. Middleburgh, R. W. Grimes, and U. Schwingenschlögl, “Extreme Palladium Diffusion in Germanium,” *J. Mater. Chem. A* **3**, 3832-3838 (2015).
13. E. E. Jay, M. J. D. Rushton, **A. Chroneos**, R. W. Grimes, and J. A. Kilner, “Genetics of Superionic Conductivity in Lithium Lanthanum Titanates,” *Phys. Chem. Chem. Phys.* **17**, 178-183 (2015).
14. M. J. D. Rushton and **A. Chroneos**, “Impact of Uniaxial Strain and Doping on Oxygen Diffusion in  $CeO_2$ ,” *Sci. Rep.* **4**, 6068 (2014).
15. **A. Chroneos** and H. Bracht, “Diffusion of n-Type Dopants in Germanium,” *Appl. Phys. Rev.* **1**, 011301 (2014) (inaugural issue).
16. R. V. Vovk, N. R. Vovk, O. V. Shekhovtsov, I. L. Goulatis, and **A. Chroneos**, “C-Axis Hopping Conductivity in Heavily Pr-Doped YBCO Single Crystals,” *Supercond. Sci. Technol.* **26**, 085017 (2013).
17. **A. Chroneos**, B. Yildiz, A. Tarancon, D. Parfitt, and J. A. Kilner, “Oxygen Transport in SOFC Cathode and Electrolyte Materials” *Energy Environ. Sci.* (invited feature article) **4**, 2774 (2011).



18. **A. Chroneos**, C. A. Londos, E. N. Sgourou, and P. Pochet, “*Point Defect Engineering Strategies to Suppress A-Center Formation in Silicon*,” *Appl. Phys. Lett.* **99**, 241901 (2011).

19. **A. Chroneos**, D. Parfitt, J. A. Kilner, and R. W. Grimes, “*Anisotropic Oxygen Diffusion in Tetragonal  $La_2NiO_{4+\delta}$ : Molecular Dynamics Calculations*,” *J. Mater. Chem.* **20**, 266-270 (2010).

20. **A. Chroneos**, H. Bracht, R. W. Grimes, and B. P. Uberuaga, “*Vacancy-Mediated Impurity Diffusion in Germanium*,” *Appl. Phys. Lett.* **92**, 172103 (2008).

### **Chapters in Books**

1. **A. Chroneos**, “*Computational Study of Energy Materials*”. In: N. Pryds and V. Espisito (eds.) “*Metal Oxide-Based Thin Film Structures*”, 263-281, 2017, Elsevier (Amsterdam).

2. **A. Chroneos**, M. J. D. Rushton, and R. W. Grimes, “*Fundamental Point Defect Properties in Ceramics*”. In: R. J. M. Konings (ed.) “*Comprehensive Nuclear Materials*”, Volume **1**, 46-64, 2012, Elsevier (Amsterdam).

3. **A. Chroneos**, C. L. Bishop, D. C. Parfitt, and R. W. Grimes, “*Atomic-Scale Computer Simulation of Functional Materials: Methodologies and Applications*”. In: J. A. Kilner, S. J. Skinner, S. J. C. Irvine, and P. P. Edwards (eds.) “*Functional Materials for Sustainable Energy Applications*”, 643-661, 2012, Woodhead Publishing (Cambridge).

## **10 REFEREES**

### **Sir Robin W. Grimes FRS FREng**

Professor in Materials Physics  
Dept. of Materials  
Imperial College London  
London SW7 2AZ  
United Kingdom  
Tel: 207-5946730  
Email: r.grimes@imperial.ac.uk

### **Prof. Lefteri H. Tsoukalas**

School of Nuclear Engineering  
Purdue University  
West Lafayette IN 47907  
USA  
Tel: +1-765-496-9696  
Email: tsoukala@purdue.edu