José D. Querales

Postdoctoral Researcher

Materials Theory Group
Tyndall National Institute
Lee Maltings, Cork T12 R5CP, Ireland
(+353)-(0)21 2346280
jose.querales@tyndall.ie

Personal data

Date of birth: 20/4/1986
Nationalities: Argentinian/Venezuelan
Country of residence: Ireland (Since March 2017)

Field of Research

Computational/Theoretical physicist, interested on the effects of electron-electron and electron-phonon scattering on the transport, thermoelectric and optical properties of novel materials of interest for technological applications, using simplified models for their description and appropriate numerical and analytical techniques to treat the effects of disorder and of correlations.
Keywords: Condensed matter physics, First-principles electronic structure calculations, Electron-electron correlations, Electron-phonon interaction, Thermoelectric materials.

Education

2011–2016 **Doctor in Physics**, *Balseiro Institute - National University of Cuyo*, Argentina.

Dissertation: Electronic properties of novel materials: alloys for nanoelectronic, superconductors based on Fe, and based on BiS_2.

Advisor: Prof. Dr. Cecilia I. Ventura (CONICET-Argentina, UNRN)

Thesis grade: Outstanding (10/10).

2009–2010 **Master in Physical Sciences**, *Balseiro Institute - National University of Cuyo*, Argentina.

Degree work: Semiconductor alloys with adjustable gap: electronic structure of $Ge_{1-x}Sn_x$.

Advisors: Prof. Dr. Cecilia I. Ventura (CONICET-Argentina, UNRN) and Prof. Dr. Rafael A. Barrio (UNAM-Mexico).

2003–2009 **Bachelor's Degree (Licenciado en Física)**, *University of Carabobo*, Venezuela.

Degree work: Preparation and characterization of Fe-Ge alloys.

Advisors: Prof. Angel E. Rivas (University of Carabobo, Venezuela) and Prof. Fernando Gonzalez† (Central University of Venezuela).

Postdoctoral Research Appointments

March 2017–Present **Postdoctoral Researher**, *Materials Theory Group, Tyndall National Institute, University College Cork*, Ireland.

Supervisors: Dr. Ivana Savić and Prof. Stephen Fahy.

Project: Theory and simulation of thermoelectric materials near structural phase transitions (Funded by Science Foundation Ireland).

Apr. 2016–Feb. 2017 **Postdoctoral Fellow**, *Surface Physics Group, Bariloche Atomic Centre*, Argentina.

Supervisors: Dr. Javier D. Fuhr and Dr. Cecilia I. Ventura.

Project: Effects of the presence of non-substitutional complex defects on the electronic properties of semiconductor alloys, and other materials of interest (Funded by the National Scientific Research Council of Argentina).

Postdoc Research Collaborations

- **Northern Ireland:** Dr. Pablo Aguado-Puente (Postdoc), Dr. Piotr Chudzinski (Postdoc), Dr. Tchavdar Todorov (Reader), Dr. Myrta Grüning (Senior Lecturer), Prof. Jorge Kohanoff (Professor) at Atomistic Simulation Centre, Queen's University Belfast.
  Topics: Many-Body Perturbation Theory (GW) calculations, theory of electron-phonon interaction and termoelectric transport properties.
- **China**: Prof. Jiang Cao, Associate Professor at Nanjing University of Science and Technology.
  Topic: Theory and simulation of thermoelectric properties of materials near phase transitions.
- **England**: Dr. Éamonn Murray, Department of Materials, Imperial College London. Topic: First principles simulation of photoexcitation in solids.
- **United States**: Experimental collaboration with Prof. Davis Reis (Stanford University), Dr. Jonathan Sobota (SLAC National Accelerator Lab), and Samuel Teitelbaum (Arizona State Univ.)
  Topics: Ultrafast dynamics in solids, Time-resolved ARPES, and X-ray experiments.
- **Italy**: Prof. Roberta Citro (Dipartimento di Fisica "E.R. Caianiello" Università degli Studi di Salerno)
  Topics: Theory of spectral properties and transport in unconventional superconductors.
- **Argentina**: Dr. Javier Fuhr (Instituto de Física del Sur, Bahia Blanca)
  Topics: First principles theory of defects in semiconductors.
  Dr. Cecilia I. Ventura (Centro Atómico Bariloche and Univ. Nacional de Río Negro)
  Topics: Theory of defects in semiconductors, spectral properties and transport in unconventional superconductors.

Fellowships and Awards

- **2019**, Irish Center for High End Computing (ICHEC) class B project #tiphy054b: "First-principles calculation of phonon-limited carrier mobility in the topological insulator SnTe" (Principal Investigator, 1,000,000 core hours).
- **2019**, Irish Center for High End Computing (ICHEC) class C project #tiphy050c: "Electron-phonon coupling in the photoexcited topological insulator Bi_2Te_3" (Principal Investigator, 100,000 core hours).
- **2016**, Postdoctoral fellowship from the National Scientific Research Council of Argentina to support my research project: "Effects of the presence of non-substitutional complex defects on the electronic properties of semiconductor alloys, and other materials of interest" at Bariloche Atomic Centre, Argentina.
- **2014**, Doctoral fellowship (type II) from the National Scientific Research Council of Argentina to support my PhD studies at Balseiro Institute, Argentina.
- **2011**, Doctoral fellowship (type I) from the National Scientific Research Council of Argentina to support my PhD studies at Balseiro Institute, Argentina.
- **2009**, joint Balseiro Institute and International Centre of Theoretical Physics Postgraduate Diploma Program Fellowship.
- **2007**, Gran Mariscal de Ayacucho Foundation, Venezuelan Ministry of Science fellowship.

Teaching Experience

Feb. 2016 – Dec. 2017 **Teaching Assistant-I (Ayudante de primera categoria)**, *Balseiro Institute, National University of Cuyo, Argentina.*

Undergraduate courses: 2 courses, Physics and Engineering careers: Introduction to Solid State Physics (Prof. Gonzalo Usaj, *February-July 2016*), Classical Mechanics (Prof. Guillermo Abramson, *August-December 2016*)

October 2013 **Teaching Assistant**, *at Balseiro Institute-Bariloche Atomic Centre School "José A. Balseiro": electrons, light and sound in nanostructures: from the fundamentals to devices.*

Subject: Electronic properties of confined systems and superlattices (Prof. Cesar Proetto)

April 2009 – July 2009 **Instructor**, *at National University of the Armed Forces (UNEFA), Venezuela.*

Subject: Thermodynamics

March 2009 – July 2009 **Instructor**, *at University Institute of Technology "Antonio José de Sucre", Venezuela.*

Subjects: General Physics, Electronic, Thermodynamics

Oct. 2008 – April 2009 **Instructor**, *at University Institute of Technology "Antonio José de Sucre", Venezuela.*

Subjects: General Physics, Electronic, Metallurgy

Jan. 2008 – April 2009 **Undergraduate Teaching Assistant**, *at Department of Physics of University of Carabobo, Venezuela.*

Subjects: Waves and Optics Lab, Electronic Lab

Supervision Experience

- Since April 2019, I have been involved in the supervision of the Ph.D. student Shima Sharifi (her Ph.D. supervisors are Dr. Ivana Savić and Prof. Stephen Fahy).
- In 2019, I was involved in the supervision of Mr. Robert Power's summer project: "Surface and Bulk Vibrational Modes in a Photo-Excited Topological Insulator Bi_2Te_3", under the supervision of Prof. Stephen Fahy.
- In 2020, I participated in the supervision of Miss. Meabh Allen's final year project: "Surface vibrational modes in Bi_2Te_3 and Bi_2Se_3, two layered topological insulators.", under the supervision of Prof. Stephen Fahy.

Postgraduate courses

During my studies at Balseiro Institute I took postgraduates courses in advanced topics on theoretical, computational and phenomenological condensed matter physics, as listed below:

Master in Physical Sciences (Balseiro Institute, Bariloche - Argentina)

Solid State Physics (2009) | Phenomenology of condensed matter (2009)| Linear response and introduction to the Green's functions (2010) | Phase transitions and critical phenomena (2010) | Magnetism (2010) | Phenomenology of Superconductivity (2010) | Interaction of photons and particles with condensed matter (2010).

Ph.D. Courses (Balseiro Institute, Bariloche - Argentina)

Crystal structure and defects in solids (2011) | Mesoscopics and nanostructured systems: magnetic properties in nanostructured systems (2012) | Many body theories in solids (2012) | Computational Physics (2012) | Advanced Topics on Computational Physics (2012) | Course on Density Functional Theory (2014).

Graduate Courses Average Grade: 9.18 (over a maximum of 10)

Publications in peer-reviewed scientific journals

1. *Electron-phonon interactions and high thermoelectric figure of merit in n-type PbTe driven towards second-order structural phase transition from first principles*,
   J. Cao, D. Dangić, **J. D. Querales-Flores**, S. Fahy and I. Savić.
   To be submitted (2020).
2. *Electron-phonon scattering and thermoelectric transport in p-type PbTe from first principles*,
   R. D'Souza, J. Cao, **J. D. Querales-Flores**, S. Fahy and I. Savić.
   Under review (2020).
3. * *Towards temperature-induced topological phase transition in SnTe: A first principles study*,
   J. D. Querales-Flores, P. Aguado-Puente, D. Dangić, J. Cao, P. Chudzinski, T. N. Todorov, M. Grüning, S. Fahy and I. Savić.
   Phys. Rev. B 101, 235206 (2020).
4. * *Thermally induced band gap increase and high thermoelectric figure of merit of n-type PbTe*,
   J. Cao, **J. D. Querales-Flores**, S. Fahy and I. Savić.
   Mater. Today Phys. (2019), DOI: https://doi.org/10.1016/j.mtphys.2019.100172.
5. * *Ultrafast relaxation of symmetry-breaking photo-induced atomic forces*,
   S. O'Mahony, F. Murphy-Armando, E. D. Murray, **J. D. Querales-Flores**, I. Savić, S. Fahy.
   Phys. Rev. Lett. 123, 087401 (2019).
6. *Effect of N interstitial complexes on the electronic properties of $GaAs_{1-x}N_x$ alloys from first principles*,
   J. D. Querales-Flores, C.I. Ventura and J. D. Fuhr.
   Phys. Rev. Materials 3, 024602 (2019).
7. * *Temperature effects on the electronic band structure of PbTe from first principles*,
   J. D. Querales-Flores, J. Cao, S. Fahy and I. Savić.
   Phys. Rev. Materials 3, 055405 (2019).
8. * *Dominant electron-phonon scattering mechanisms in n-type PbTe from first principles*,
   J. Cao, **J. D. Querales-Flores**, A. R. Murphy, S. Fahy and I. Savić.
   Phys. Rev. B 98, 205202 (2018).
9. * *The two gap transitions in $Ge_{1-x}Sn_x$: effect of non-substitutional complex defects*,
   J. D. Querales-Flores, C.I. Ventura, J. D. Fuhr and R. A. Barrio.
   J. Appl. Phys. 120, 105705 (2016).
10. *Temperature and doping dependence of normal state spectral properties in a two-orbital model for ferropnictides*
    J. D. Querales-Flores, C. I. Ventura, R. Citro and J.J. Rodríguez-Núñez.
    Phys. Lett. A 380, 1648-1657 (2016).
11. *Normal state electronic properties of $LaF_xO_{1-x}BiS_2$ superconductors*,
    J. D. Querales-Flores, C. I. Ventura, R. Citro and J.J. Rodríguez-Núñez.
    Physica B: Condensed Matter 488, 32-42 (2016).
12. *Normal state magnetotransport properties of β-FeSe superconductors*,
    J. D. Querales-Flores, M. L. Amigó, G. Nieva and C. I. Ventura.
    Europhys. Lett. 113, 17005 (2016).
13. * *Electronic structure of $Ge_{1-x-y}Si_xSn_y$ ternary alloys for multijunction solar cells*,
    C.I. Ventura, **J. D. Querales-Flores**, J.D. Fuhr and R.A. Barrio.
    Prog. Photovolt: Res. Appl. 23, 112 - 118 (2015).
14. *Non-substitutional Sn Defects in $Ge_{1-x}Sn_x$ alloys for Opto- and Nanoelectronics*,
    R. A. Barrio, **J. D. Querales-Flores**, J. D. Fuhr and C. I. Ventura.
    J. of Superc. and Novel Magn. 26, 2213-2217 (2013).

Peer-review service

- Reviewer for: MDPI Materials, MDPI Applied Sciences and Journal of Applied Physics.

Invited talks

- **2019**: "Temperature effects on the electronic structure of the weak topological insulator SnTe". ASC-CTAMOP Seminar Series at Queen's University Belfast, United Kingdom.
- **2014**: "Electronic structure of $Ge_{1-x-y}Si_xSn_y$ ternary alloys for high efficiency solar cells and optoelectronic". Department of Physics - FACYT, University of Carabobo. Venezuela.

International Conferences

Oral Presentations

1. "Phonon-induced topological phase transition in SnTe". Accepted to be presented at the American Physical Society (APS) March Meeting 2020. March 2020; Denver, Colorado, USA. (**Collaboration with Queen's University Belfast**).
2. "Temperature dependence of electronic structure and electron-phonon coupling in the weak topological insulator SnTe". "2019 European Materials Research Society Spring Meeting". May 2019; Nice, France.
3. "Temperature effects on the electronic band structure of PbTe from first principles". American Physical Society (APS) March Meeting 2019; Boston, Massachusetts, USA.
4. "Electron-phonon coupling in photoexcited Bi_2Te_3". American Physical Society (APS) March Meeting 2019. March 2019; Boston, Massachusetts, USA. (**Experimental collaboration with Stanford University**).
5. "Electron-phonon coupling at the surface state of the topological insulator Bi_2Te_3". First general meeting COST action 17126. November 2018; Madrid, Spain. (**Experimental collaboration with Stanford University**).
6. "Temperature effects on the electronic band structure of PbTe from first principles". 18^{th} IEEE International Conference on Nanotechnology. July 2018; Cork, Ireland.
7. "Electron-phonon coupling and thermoelectric transport in n-type PbTe". 2018 European Materials Research Society Spring Meeting. June 2018; Strasbourg, France.
8. "Temperature effects on the electronic band structure of PbTe from first principles". Nanoscale Simulators of Ireland Annual Meeting. May 2018; Bernal Institute, Limerick, Ireland.

Poster Presentations

1. "Electron-phonon scattering in n-type PbTe from first principles calculations", J. Cao, **J. D. Querales-Flores**, R. Murphy, S. Fahy and I. Savić. 2018 ICTP/Psi-k/CECAM School on Electron-Phonon Physics from First Principles. The Abdus Salam International Centre for Theoretical Physics. Trieste, Italy, March 2018.
2. "Temperature variation of electronic structure of n-type PbTe and its impact on thermoelectric transport", **J. D. Querales-Flores**, J. Cao, R. Murphy, S. Fahy and I. Savić. 2018 ICTP/Psi-k/CECAM School on Electron-Phonon Physics from First Principles. The Abdus Salam International Centre for Theoretical Physics, Trieste - Italy, March 2018.
3. "Normal state magnetotransport properties of β-FeSe superconductors", **J. D. Querales-Flores**, M.L. Amigó, G. Nieva and C.I. Ventura. Workshop on "Fermi-Surface Topology and Emergence of Novel Electronic States in Strongly Correlated Systems and Interference and Magnetism and Superconductivity". International Institute of Physics, Natal/RN - Brazil, July 2016.
4. " The two gap transitions in $Ge_{1-x}Sn_x$: effect of non-substitutional complex defects", Cecilia I. Ventura, **J. D. Querales-Flores**, J. D. Fuhr and R. A. Barrio. Gordon Research Conference "Defects in Semiconductors". Bentley University, Waltham, Boston, MA, U.S.A. August 2014 (Presented by C.I. Ventura).
5. " Temperature and doping dependence of the electronic structure of ferropnictides", **J. D. Querales-Flores**, C.I. Ventura, R. Citro and J.J. Rodríguez-Núñez. Workshop on "Quantum Criticality in Correlated Materials and Model Systems". International Institute of Physics,

Natal/RN - Brazil, July, 2014.

6. "Electronic structure of $Ge_{1-x-y}Si_xSn_y$ ternary alloys", C. I. Ventura, **J. D. Querales-Flores**, R. A. Barrio, J. D. Fuhr. Gordon Research Conference "Defects in Semiconductors", Biddeford, Maine 2012 (Presented by C.I. Ventura).
7. "Inclusion of non-substitutional defects in electronic structure calculations: application to $Ge_{1-x}Sn_x$" **J. D. Querales-Flores**, C. I. Ventura, J. D. Fuhr and R. A. Barrio. 16th International Conference: "Recent Progress in Many-Body Theories" San Carlos de Bariloche - Argentina, December 2011.
8. " Non-substitutional defects in the electonic structure of $Ge_{1-x}Sn_x$", **J. D. Querales-Flores**, C. I. Ventura XII Giambiagi School: "Low dimensional condensed matter", Buenos Aires - Argentina, July 2010.

Participation in International Schools/Workshops

- 2018 ICTP/Psi-k/CECAM School on Electron-Phonon Physics from First Principles. Trieste, Italy, March 2018 (Selected by organizers).
- Questaal Suite hands on workshop. Daresbury Laboratory. Warringston, United Kingsdom, May 2017 (Selected by organizers: *full travel grant awarded*).
- Fermi-Surface Topology and Emergence of Novel Electronic States in Strongly Correlated Systems and Interference and Magnetism and Superconductivity. International Institute of Physics, Natal/RN, Brazil, July 2016 (Selected by organizers: *full travel grant awarded*).
- School on "Electronic Structure and Quantum Transport Methods". International Centre for Theoretical Physics-South American Institute for Fundamental Research (ICTP-SAIFR. Sao Paulo, Brazil, October 2014 (Selected by organizers: *full travel grant awarded*).
- Workshop on Quantum Criticality in Correlated Materials and Model Systems. International Institute of Physics, UFRN. Natal/RN, Brazil, July 2014 (Selected by organizers: *full travel grant awarded*).
- 6th I2CAM-FAPERJ Spring School "New Perspectives in Quantum Matter". Centro Brasilero de Pesquisas Fisicas (CBPF) and Institute for Complex Adaptative Matter (ICAM-I2CAM). Río de Janeiro, Brazil, April 2013 (Selected by organizers: *full travel grant awarded*).
- ANDES / ALPS School "School on numerical methods for many-body theories". Bariloche Atomic Center, Bariloche, Argentina, December 2011.
- Eulasur Summer School and Workshop "Simulation, characterization and optical methods for materials and nanomaterials". La Plata, Argentina, September 2011 (Selected by organizers: *full travel grant awarded*).
- Eulasur Summer School and Workshop "Properties and applications of nanomaterials". Bariloche Atomic Center, Bariloche, Argentina, October 2010.
- XII Giambiagi School "Low dimensional condensed matter". University of Buenos Aires. Buenos Aires, Argentina, July 2010.

Scientific Internships

Aug. 2007 – Oct. 2007 **Visiting student**, *Condensed Matter Physics Lab - Institute for Scientific Research, Caracas, Venezuela. Advisor: Dr. Pedro Silva..*

July 2008 – July 2009 **Assistant student**, *Science and Engineering of Materials Lab, Materials Engineering and Nanotechnology Center, Institute for Scientific Research, Caracas, Venezuela. Advisor: Dr. Gema Gonzalez..*

Languages

* Spanish: Mother tongue.

* General English fluency course at The Language Centre, University College Cork, Ireland - At level B2 (Common European Framework Reference), April to June, 2017.

* English: Upper-intermediate level: B2 Common European Framework of Reference for Languages (CEFR). First Certificate in English, University of Cambridge, August 2018.

Highlight of skills

* Experience in scientific programming and data analysis (C/C++, FORTRAN, Python).
* I have worked extensively with the ABINIT, VASP, EPW (electron-phonon Wannier) and Quantum-ESPRESSO density functional theory ab-initio packages for carrying out calculations during my research.

Professional development and training

- Python Programmer Track (52 hours). Datacamp online platform (2019).
- Course: Research Integrity Epigeum. June 2019.
- Workshop: Effective Networking. University College Cork. October 2018.
- Course: Addressing Dissemination, Communication and Outreach in Research Proposals. University College Cork. April 2018.
- Course: Proposal Writing and Costing Workshop. University College Cork. February 2018.

Further Academic/related activities

1. Member of the American Physical Society, since November 2018.
2. Member of the European Materials Research Society, since June 2018.
3. Member of the Surface Physics Group - Centro Atómico Bariloche (04/2016 - 02/2017). Postdoctoral fellow.
4. Member of the Solid State Theory Group - Centro Atómico Bariloche (from 08/2009 - 03/2016). PhD. Student.
5. Member of the Argentinian Physics Association, (07/2011-07/2016).

Academic References

- **Dr. Ivana Savić**
  Research Scientist, Tyndall National Institute, Cork (T12R5CP), Ireland. **e-mail**: ivana.savic@tyndall.ie
- **Prof. Stephen Fahy**
  Associate Professor, Department of Physics, University College Cork, Cork (T12K8AF), Ireland. **e-mail**: s.fahy@ucc.ie
- **Prof. Jorge Kohanoff**
  Professor, School of Mathematics and Physics, Atomistic Simulation Centre, Research Centre in Sustainable Energy, Queen's University Belfast, United Kingdom. **e-mail**: j.kohanoff@qub.ac.uk
- **Dr. Tchavdar Todorov**
  Reader, School of Mathematics and Physics and Atomistic Simulation Centre, Queen's University Belfast, United Kingdom. **e-mail**: t.todorov@qub.ac.uk
- **Dr. Javier D. Fuhr**
  Investigador Independiente, National Scientific Research Council of Argentina (CONICET), Instituto de Física del Sur, Bahía Blanca, Argentina.
  e-mail: javier.fuhr@gmail.com
- **Prof. Cecilia I. Ventura**
  Associate Professor, National University of Río Negro, (8400) Bariloche, Argentina.
  Investigador Adjunto, National Scientific Research Council of Argentina (CONICET), Bariloche Atomic Center, (8400) Bariloche, Argentina.
  e-mail: ventura@cab.cnea.gov.ar, civenturaschroeder@gmail.com