David Jacob

Curriculum Vitae

Universidad del País Vasco
Departamento de Física de Materiales
Avenida de Tolosa 72
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Professional Appointments

Universidad del País Vasco — **San Sebastian, Spain**
Ikerbasque Research Fellow, Departamento de Física de Materiales — *Since Apr. 2017*
Research: *Electronic correlations and spin dynamics in nanoscale quantum systems*

Max-Planck-Institut für Mikrostrukturphysik — **Halle, Germany**
Postdoctoral Researcher, Theory Department (Prof. E. K. U. Gross) — *Nov. 2009 – Mar. 2017*
Research: *Ab initio theory of strongly correlated materials and nanostructures*

Universität Hamburg — **Hamburg, Germany**
Visiting Scientist, I. Institut für Theoretische Physik — *Oct. 2009*
Group of Prof. A. I. Lichtenstein

Rutgers - The State University of New Jersey — **Piscataway, NJ USA**
Postdoctoral Associate, Department of Physics & Astronomy — *Sep. 2007 – Sep. 2009*
Advisor: Prof. Gabriel Kotliar
Research: *Dynamical Mean-Field Theory for strongly correlated materials and nanostructures*

Education

Universidad de Alicante — **Alicante, Spain**
PhD Physics, Grade: *sobresaliente cum laude* — *Mar. 2003 – May 2007*
Dissertation: *Spin transport in nanocontacts and nanowires*
Advisor: Prof. Juan-José Palacios

Universität Hamburg — **Hamburg, Germany**
Diplom-Physiker (MSc Physics), Grade: *ausgezeichnet (excellent)* — *Oct. 1996 – Jul. 2002*
Diploma Thesis: *Elektronische Struktur gekoppelter Quantenpunkte*
Supervisor: Prof. Daniela Pfannkuche

University of Southampton — **Southampton, UK**
Year abroad, Erasmus programme, Department of Physics & Astronomy — *Sep. 1998 – Jun. 1999*

Research Highlights

- 9 years of Postdoc experience in the US and Germany
- Over 40 indexed publications, including Nature (2), Nature Nanotechnology (1), Nano Letters (3), Physical Review Letters (4)
- Over 1300 citations, Hirsch index h=19 (Google Scholar)
- 3 single author publications (J. Phys. Condens. Matter 2015 & 2018 and Phys. Rev. B 2018)
- Over 30 invited talks and research seminars
- Main organizer of "What about U?" Workshop, Zaragoza, May 21-24, 2019
- Co-organizer of "What about U?" Workshop at ICTP Trieste, October 17-21, 2016
- Developer of ab initio quantum transport codes ANT.G and ANT.1D, www.simuneatomistics.com/ant
- Inventor of NanoDMFT method (PRL 2009 and PRB 2010)

Current Research Interests

- Strong electronic correlations in nanoscale devices, molecules and solids
- Kondo effect and spin excitations of nanoscale quantum magnets
- Quantum transport through nanoscale junctions
- Foundations of density functional theory
- Dynamical mean-field theory and impurity solver development

Most Cited Publications

- *Coherent transport in graphene nanoconstrictions* **(191 citations)**
  F. Muñoz-Rojas, D. Jacob, J. Fernández-Rossier and J. J. Palacios, Phys. Rev. B **74** 195417 (2006)
- *The Kondo effect in ferromagnetic atomic contacts* **(162 citations)**
  M. R. Calvo, J. Fernández-Rossier, J. J. Palacios, D. Jacob, D. Natelson, and C. Untiedt
  Nature **458** 1150 (2009)
- *Control of single-spin magnetic anisotropy by exchange coupling* **(126 citations)**
  J. C. Oberg, M. R. Calvo, F. Delgado, M. Moro-Lagares, D. Serrate, D. Jacob, J. Fernández-Rossier, C. F. Hirjibehedin, Nature Nanotech. **9** , 64 (2014)
- *Orbital selective and tunable kondo effect of magnetic adatoms on graphene* **(91 citations)**
  D. Jacob and G. Kotliar, Phys. Rev. B **82**, 085423 (2010)
- *Dyanmical mean-field theory for molecular electronics* **(73 citations)**
  D. Jacob, K. Haule, and G. Kotliar, Phys. Rev. B **82**, 195115 (2010)
- *Kondo effect and conductance of nanocontacts with magnetic impurities* **(68 citations)**
  D. Jacob, K. Haule and G. Kotliar, Phys. Rev. Lett. **103**, 016803 (2009)
- *Magnetic and orbital blocking in ni nanocontacts* **(68 citations)**
  D. Jacob, J. Fernández-Rossier, and J. J. Palacios, Phys. Rev. B **71**, 220403(R) (2005)
- *Transport in magnetically ordered Pt nanocontacts* **(48 citations)**
  J. Fernández-Rossier, D. Jacob, C. Untiedt, and J.J. Palacios, Phys. Rev. B **72**, 224418 (2005)
- *Kondo effect and spin quenching in high-spin molecules on metal substrates* **(47 citations)**
  D. Jacob, M. Soriano, and J.J. Palacios, Phys. Rev. B **88**, 134417 (2013)
- *Towards a full ab initio theory of strong electronic correlations in nanoscale devices* **(44 citations)**
  D. Jacob, J. Phys.: Condens. Matter **27**, 245606 (2015)

Teaching Experience

Introduction to Dynamical Mean-Field Theory — **DIPC, San Sebastian**
DIPC Lectures — *Nov-Dec 2018*

Computational Physics — **MLU Halle-Wittenberg**
BSc. Physics course — *Winter 2015*

Advanced Solid State Physics — **MLU Halle-Wittenberg**
MSc. Physics course — *Summer 2013*

The Kondo Effect in Metals and Nanostructures — **MPI Halle**
IMPRS Graduate School — *Winter 2012*

Introduction to Quantum Many-Body Physics — **MPI Halle**
IMPRS Graduate School — *Summer 2012*

Supervision of PhD students
Sebastian Frank (MPI Halle) — *Jun. 2012 - Aug. 2020*
Sareh Motahari (MPI Halle) — *Sep. 2012 - Aug. 2017*

Awards and Fellowships

IKERBASQUE Foundation — **Spain**
IKERBASQUE Research Fellowship — *Jul. 2016*

Deutscher Akademischer Austauschdienst (DAAD) — **Germany**
Postdoc scholarship — *2008 – 2009*

Ministerio de Educación y Ciencia (MECD) — **Spain**
PhD scholarship — *2004 – 2007*

Universidad de Murcia — **Spain**
Scholarship for Research Collaboration — *2003*

Phantoms Foundation — **Spain**
TNT 2003 Poster Award — *Sep. 2003*

Funding

Ministerio de Ciencia y Inovación, *Generación de Conocimiento Call 2020* — Sep. 2021 – Aug. 2024
Project: QuEST - *Quantum Theory of Electron, Spin and Thermal Transport* — Role: **Co-PI**
Ref.: PID2020-112811GB-I00 — Amount: **104060€**

Gobierno Vasco, *Grupos Consolidados Call 2019* — Jan. 2019 – Dec. 2021
Project: FunTheMaS - *Fundamental Theoretical Materials Science* — Role: **Research team**
Ref.: IT1249-19 — Amount: **325500€**

CECAM, *Workshop Funding Call 2018* — May 2019
Workshop: *What about U in nanoscale systems?* — Role: **Main Organizer**
Ref.: 1677 — Amount: **4000€**

Psi-K Foundation, *Workshop Funding Call 2018* — May 2019
Workshop: *What about U in nanoscale systems?* — Role: **Main Organizer**
Amount: **6000€**

Organization of Scientific Events

What about U in nanoscale systems? — **ZCAM, Zaragoza**
CECAM Workshop, Role: Main Organizer — *May 2019*

What about U? Effects of Hubbard Interactions and Hund's Coupling in Solids — **ICTP, Trieste**
CECAM Workshop, Role: Co-organizer — *Oct 2016*

Additional Qualifications

April 2018: ANECA "Profesor Contratado Doctor" certificate

Languages

German native language
English fluent (speaking, reading, writing)
Spanish fluent (speaking, reading, writing)

Other Merits

Referee for Nature Physics, Nature Communications, Proceedings of National Academy of Sciences, Nano Letters, Physical Review Letters, Physical Review B and A, Journal of Physics: Condensed Matter, and Europhysics Letters.

Employment outside Academia

Hamburg-Consult **Hamburg (Germany)**
Programmer (C, C++) *Sep. 1996 – Dec. 2002*
Student part time job; software development for public transportation companies

Philips Research Laboratories **Hamburg (Germany)**
Internship *Feb.-Mar. 2000*
Software development for automatic image recognition in medical applications

Military Service

1995 – 1996: 3 months basic army training; 7 months orderly at Führungsakademie der Bundeswehr

References

- **Prof. Dr. Eberhard Gross**
  Max-Planck-Institut für Mikrostrukturphysik, Theorie-Abteilung
  Weinberg 2, 06120 Halle (Germany)
  email: ekugross@mpi-halle.mpg.de
  phone: (+49) (0)345 / 5582-763
- **Prof. Dr. Gabriel Kotliar**
  Rutgers University, Department of Physics & Astronomy
  136 Frelinghuysen Road, Piscataway, NJ 08854-8019 (USA)
  email: kotliar@physics.rutgers.edu
  phone: (+1) 732 / 445-5500-4331
- **Prof. Dr. Joaquin Fernández-Rossier**
  INL | International Iberian Nanotechnology Laboratory
  Av. Mestre José Veiga, 4715-310 Braga, Portugal
  & Dpto. de Fśica Aplicada, Universidad de Alicante
  San Vicente del Raspeig, Spain
  email: joaquin.fernandez-rossier@inl.int & jfrossier@ua.es
  phone: (+351) 253 090 612 (INL) & (+34) 965903541 (Univ. Alicante)
- **Prof. Dr. Juan José Palacios**
  Universidad Autónoma de Madrid, Dpto. de la Física de la Materia Condensada
  Facultad de Ciencias, C03, Campus de Cantoblanco, Madrid 28049 (Spain)
  email: juanjose.palacios@uam.es
  phone: (+34) 91497-6416

Publications

Summary: 42 indexed publications, including Nature (2), Nature Nanotechnology (1), Nano Letters (3), and Physical Review Letters (4), Physical Review B (19), Journal of Chemical Physics (2), EPL (1); over 1300 citations, Hirsch index h=19 (Google Scholar)

Regular Articles

- *Observation of fractional edge excitations in nanographene spin chains*
  S. Mishra, G. Catarina, F. Wu, R. Ortiz, D. Jacob, K. Eimre, J. Ma, C.A. Pignedoli, X. Feng, P. Ruffieux, J. Fernández-Rossier, and R. Fasel
  accepted in Nature (Jul. 2021), preprint at arXiv:2105.09102
- *Mott metal-insulator transition from steady-state density functional theory*
  D. Jacob, G. Stefanucci, and S. Kurth

Phys. Rev. Lett. **125**, 216401 (2020)

- *Exchange correlation potential for the multi-orbital Anderson impurity model*
  N. Sobrino, S. Kurth and D. Jacob
  Phys. Rev. B **102**, 035159 (2020)
- *Spin dependent transmission of nickelocene-Cu contacts probed with shot noise*
  M. Mohr, M. Gruber, A. Weismann, D. Jacob, P. Abufager, N. Lorente, and R. Berndt
  Phys. Rev. B **101**, 075414 (2020)
- *Nonequilibrium spectral functions from multiterminal steady-state density functional theory*
  S. Kurth, D. Jacob, N. Sobrino, and G. Stefanucci
  Phys. Rev. B **100**, 085114 (2019)
- *Electrically addressing the spin of a magnetic porphyrin through covalently connected graphene electrodes*
  J. Li, N. Friedrich, N. Merino, D. G. de Oteyza, D. Peña, D. Jacob, and J. I. Pascual
  Nano Lett. **19**, 3288 (2019)
- *Simulation of inelastic spin flip excitations and Kondo effect in STM spectroscopy of magnetic molecules on metal substrates*
  D. Jacob
  J. Phys.: Condens. Matter **30**, 3554003 (2018)
- *Exchange-correlation functionals of i-DFT for asymmetrically coupled leads*
  S. Kurth and D. Jacob
  Euro. Phys. J. B **91**, 101 (2018)
- *Renormalization of single-ion magnetic anisotropy in the absence of the Kondo effect*
  D. Jacob
  Phys. Rev. B **97**, 075428 (2018)
- *Many-body spectral functions from steady state density functional theory*
  D. Jacob and S. Kurth
  Nano Lett. **18**, 2086 (2018)
- *Spin control induced by molecular charging in a transport junction*
  S. Karan, C. García, M. Karolak, D. Jacob, N. Lorente, and R. Berndt
  Nano Lett. **18**, 88 (2018)
- *Origin of the quasiparticle peak in the spectral density of Cr (001) surfaces*
  L. Peters, D. Jacob, M. Karolak, A. I. Lichtenstein, and M. I. Katsnelson
  Phys. Rev. B **96**, 245137 (2017)
- *Anomalous magnetism in hydrogenated graphene*
  N.A. Garcia-Martinez, J. L. Lado, D. Jacob and J. Fernández-Rossier
  Phys. Rev. B **96**, 024403 (2017)
- *Kondo physics of the Anderson impurity model by Distributional Exact Diagonalization*
  S. Motahari, R. Requist and D. Jacob
  Phys. Rev. B **94**, 235133 (2016)
- *Competition between quantum spin tunneling and Kondo effect*
  D. Jacob and J . Fernández-Rossier
  Euro. Phys. J. B **89**, 210 (2016)
- *Effects of valence, geometry and electronic correlations on transport in transition metal benzene sandwich molecules*
  M. Karolak and D. Jacob
  J. Phys.: Condens. Matter **28**, 445301 (2016)
- *Orbital signatures of Fano-Kondo lineshapes in STM adatom spectroscopy*

S. Frank und D. Jacob
Phys. Rev. B **92**, 235127 (2015)

- *Shifting the Voltage Drop in Electron Transport Through a Single Molecule*
  S. Karan, D. Jacob, M. Karolak, C. Hamann, Y. Wang, A. Weismann, A. I. Lichtenstein and R. Berndt
  Phys. Rev. Lett. **115**, 016802 (2015)
- *Towards a full ab initio theory of strong electronic correlations in nanoscale devices*
  D. Jacob
  J. Phys.: Condens. Matter **27**, 245606 (2015)
- *Control of single-spin magnetic anisotropy by exchange coupling*
  J. C. Oberg, M. R. Calvo, F. Delgado, M. Moro, D. Serrate, D. Jacob, J. Fernández-Rossier and C. F. Hirjibehedin
  Nature Nanotechnology **9**, 64 (2014)
- *Kondo effect and spin quenching in high-spin molecules on metal substrates*
  D. Jacob, M. Soriano and J. J. Palacios,
  Phys. Rev. B **88**, 134417 (2013)
- *Analysis of the Kondo effect in ferromagnetic atomic-sized contacts*
  M. R. Calvo, D. Jacob and C. Untiedt
  Phys. Rev. B **86** 075447 (2012)
- *Orbital Kondo effect in Co-benzene sandwich molecules*
  M. Karolak, D. Jacob and A. I. Lichtenstein
  Phys. Rev. Lett. **107**, 146604 (2011)
- *Critical comparison of electrode models in density functional theory based quantum transport calculations*
  D. Jacob and J. J. Palacios
  J. Chem. Phys. **134** 044118 (2011)
- *Dynamical mean-field theory for molecular electronics: Electronic structure and transport properties*
  D. Jacob, K. Haule and G. Kotliar
  Phys. Rev. B, **82**, 195115 (2010)
- *Orbital selective and tunable Kondo effect of magnetic adatoms on graphene*
  D. Jacob and G. Kotliar
  Phys. Rev. B **82**, 085423 (2010)
- *Kondo effect and conductance of nanocontacts with magnetic impurities*
  D. Jacob, K. Haule and G. Kotliar
  Phys. Rev. Lett., **103**, 016803 (2009)
- *Kondo effect in ferromagnetic atomic contacts*
  M. R. Calvo, J. Fernández-Rossier, J. J. Palacios, D. Jacob, D. Natelson and C. Untiedt
  Nature, **458**, 1150 (2009)
- *Combining the hybrid functional method with DMFT*
  D. Jacob, K. Haule and G. Kotliar
  Europhys. Lett. **84**, 57009 (2008)
- *Anisotropic magnetoresistance in nanocontacts*
  D. Jacob, J. Fernández-Rossier and J. J. Palacios
  Phys. Rev. B **77**, 165412 (2008)
- *Localized basis sets for unbound electrons in nanoelectronics*
  D. Soriano, D. Jacob and J. J. Palacios
  J. Chem. Phys. **128**, 074108 (2008)
- *Electronic structure and transport properties of atomic NiO spinvalves*

D. Jacob, J. Fernández-Rossier and J. J. Palacios
J. Magn. Magn. Mater. **310**, e675–e677 (2007)

- *Coherent transport in graphene nanoconstrictions*
  J. Fernández-Rossier J. J. Palacios F. Muñoz Rojas and D. Jacob
  Phys. Rev. B **74**, 195417 (2006)
- *Emergence of half-metallicity in suspended NiO chains*
  D. Jacob, J. Fernández-Rossier and J. J. Palacios
  Phys. Rev. B, **74**, 081402(R) (2006)
- *Orbital eigenchannel analysis for ab initio quantum transport calculations*
  D. Jacob and J. J. Palacios
  Phys. Rev. B **73**, 075429 (2006)
- *Transport through magnetically ordered Pt nanocontacts*
  C. Untiedt J. J. Palacios J. Fernández-Rossier and D. Jacob
  Phys. Rev. B **72**, 224418 (2005)
- *Magnetic and orbital blocking in Ni nanocontacts*
  D. Jacob, J. Fernández-Rossier and J. J. Palacios
  Phys. Rev. B **71**, 220403(R) (2005)
- *Isospin blockade in transport through vertical double quantum dots*
  B. Wunsch, D. Jacob and D. Pfannkuche
  Physica E **26**, 464 (2005)
- *Charge localization and isospin blocckade in vertical double quantum dots*
  D. Jacob, B. Wunsch and D. Pfannkuche
  Phys. Rev. B **70**, 081314(R) (2004)

Conference Proceedings

- *Mechanical, electrical, and magnetic properties of Ni nanocontacts*
  D. Jacob C. Untiedt, R. Calvo, A. J. Caturla, and J. J. Palacios
  IEEE Transactions on Nanotechnology, **7**, 165 (2008)
- *Mechanical and electrical properties of Ni nanocontacts*
  D. Jacob, M. J. Caturla, R. Calvo, C. Untiedt and J. J. Palacios
  Proceedings of the 2006 IEEE Nanotechnology Materials and Devices Conference **1**, 236 (2006)
- *Spin filter behaviour of atomic NiO chains in Ni nanocontacts*
  D. Jacob, J. Fernández-Rossier and J. J. Palacios
  Proceedings of the 2006 IEEE Nanotechnology Materials and Devices Conference **1**, 622 (2006)

Articles submitted or in preparation

- *Renormalization of spin excitations and Kondo effect in open shell nanographenes*
  D. Jacob, R. Ortiz, and J. Fernández-Rossier
  submitted to Phys. Rev. B. (2021), preprint at arXiv:2104.02503

Invited Talks and Seminars

Summary: 12 invited talks at international conferences and workshops; 18 invited seminars at Universities and Research Institutes

Invited talks at Conferences and Workshops

Theoretical Methods in Molecular Spintronics — **San Sebastian, Spain**
Transport signatures of complex nanoscale magnets from NanoDMFT — *Sep. 2018*

Lectiones Clitumnaliae **Campello sul Clitunno, Italy**
Many-body spectral functions from steady state density functional theory *Aug. 2018*

Magnetic Adatoms as Building Blocks for Quantum Magnetism **Mainz, Germany**
Competition between quantum spin tunneling and Kondo effect *Aug. 2015*

Electronic structure at the cutting edge with the ELK code **Lausanne, Switzerland**
DMFT - What is it? *Aug. 2015*

2nd Workshop on Fabrication and Properties of Nanostructures **Alicante, Spain**
Competition betw. Kondo effect and other quenching mechanisms in mol. devices *Jun. 2015*

IUMRS-ICYRAM 2014 Conference **Haikou, China**
Kondo effect and molecular quenching in magnetic molecules at metal substrate *Oct. 2014*

Recent progress in dynamical mean-field theory and GW calculations **Strasbourg, France**
Towards a full ab initio description of strong correlations in nanoscale devices *Dec. 2012*

GEFES'12 - VII Reunión Nacional de Física del Estado Solido **Sevilla, Spain**
Kondo effect in nanoscopic devices from first principles *Jan. 2012*

Workshop on Spin-dynamics and Kondo effects in STM **Hamburg, Germany**
Kondo effect in molecules and nanocontacts from first principles *Dec. 2011*

Workshop on strong correlations from first principles **Seeon, Germany**
COHSEX+OCA and COHSEX+DMFT for nanoscopic conductors *Aug. 2011*

Workshop on Transport Phenomena in Molecular Nanostructures **Zurich, Switzerland**
DMFT for electronic structure and transport properties of nanoscopic conductors *Jun. 2010*

Nanomediterraneo II **Alicante, Spain**
Dynamic correlations and the Kondo effect in nanostructures from first principles *Jun. 2010*

Invited Seminars at Universities and Research Institutes

Ecole Polytechnique **Paliseau, France**
Many-body spectral functions from steady-state density functional theory *Oct. 2019*
Group Seminar (Prof. Silke Biermann)

Thomas Young Centre **London, UK**
Strong correlation effects in nanoscale devices from first principles *Feb. 2017*
TYC Soiree

CIC NanoGune **San Sebastian, Spain**
Kondo effect in molecular devices from first principles *Jan. 2014*
Institute Seminar

Dpto. de Física de la Materia Condensada, Universidad Autónoma de Madrid **Madrid, Spain**
Kondo effect in molecular devices from first principles *Sep. 2013*
Department Seminar

Departamento de Física Aplicada, Universidad de Alicante **Alicante, Spain**
Kondo effect in molecular devices from first principles *Sep. 2013*
Department Seminar

Institut für Experimentalphysik, Freie Universität Berlin **Berlin, Germany**
Kondo effect in atomic- and molecular-size devices from first principles *Feb. 2011*
Group Seminar (Prof. J. I. Pascual)

Instituto de Ciencia de Materiales de Madrid (ICMM) **Madrid, Spain**
Kondo effect in molecular devices from first principles *Jan. 2011*
Institute Seminar

Instituto Madrileño de Estudios Avanzados (IMDEA) **Madrid, Spain**
Kondo effect in molecular devices from first principles *Jan. 2011*

Institute Seminar
Max-Planck-Institut für Festkörperforschung **Stuttgart, Germany**
Kondo effect in atomic-size nanostructures from first principles *Nov. 2010*
Department Seminar

Scuola Internazionale Superiore di Studi Avanzati (SISSA) **Trieste, Italy**
Kondo effect in atomic-size nanostructures with magnetic impurities *Apr. 2010*
Institute Seminar

Freie Universität Berlin **Berlin, Germany**
Kondo effect and conductance of nanocontacts with magnetic impurities *Feb. 2009*
Group Seminar (Prof. E. K. U. Gross)

Departamento de Física Aplicada, Universidad de Alicante **Alicante, Spain**
Combining hybrid functional calculations with DMFT *Jun. 2008*
Department Seminar

Dept. of Physics & Astronomy, Rutgers University **NJ Piscataway, USA**
Spin transport in nanocontacts and nanowires *Oct. 2007*
Group Seminar (Prof. G. Kotliar)

Department of Chemistry, POSTECH **Pohang, Republic of Korea**
Spin transport in nanocontacts *Oct. 2006*
Group Seminar

Korean Institute of Advanced Studies (KIAS) **Seoul, Republic of Korea**
Spin transport in nanocontacts *Oct. 2006*
Group Seminar (Prof. D. M. Kim)

I. Institut für Theoretische Physik, Universität Hamburg **Hamburg, Germany**
Magnetic and orbital blocking in Ni nanocontacts *Aug. 2005*
Institute Seminar

I. Institut für Theoretische Physik, Universität Hamburg **Hamburg, Germany**
Spin transport in nanocontacts: Theory and experiments *Aug. 2005*
Group Seminar (Prof. D. Pfannkuche)

Departamento de Física Aplicada, Universidad de Alicante **Alicante, Spain**
Magnetic-field induced charge localization in vertical double quantum dots *Apr. 2003*
Department Seminar