MINISTERIO DE CIENCIA E INNOVACIÓN

Cofinanciado por la Unión Europea

AGENCIA ESTATAL DE INVESTIGACIÓN

CURRICULUM VITAE (CVA)

IMPORTANT – The Curriculum Vitae cannot exceed 4 pages. Instructions to fill this document are available on the website.

CV date	24/11/2021

Part A. PERSONAL INFORMATION

First name	Ivo Nuno		
Family name	Saldanha do Rosário e Souza		
Gender (*)	Male	Birth date	12/03/1972
Social Security, Passport, ID number	Y1637787V (NIE)		
e-mail	ivo_souza@ehu.es	URL Web: https://cfm.ehu.es/ivo/	
Open Researcher and Contributor ID (ORCID) (*)		0000-0001-9901-5058	

(*) Mandatory

A.1. Current appointment:

Position	Ikerbasque Research Professor		
Initial date	01/01/2011		
Institution	Ikerbasque Foundation and Universidad del País Vasco		
Department/Center	Centro de Física de Materiales (CFM)	https://cfm.ehu.es/	
Country	Spain	Teleph. number	943 01 8775
Keywords	Berry phases in the band theory of solids, Wannier functions, *ab initio* calculations, topological materials, anomalous Hall effect, nonlinear optical and transport phenomena.		

A.2. Previous appointments (research activity interuptions, art. 14.2.b))

Period	Position/Institution/Country/Interruption cause
2004-2010	Assistant Professor of Physics, University of California, Berkeley
2000-2003	Postdoctoral Fellow, Department of Physics and Astronomy, Rutgers University, New Jersey

A.3. Education

Degree	University/Country	Year
PhD in Physics	University of Illinois at Urbana-Champaign	2000
Licenciatura in Physics	Universidade Técnica de Lisboa	1995

Part B. CV SUMMARY *(max. 5000 characters, including spaces)*

In the following, I refer to papers by their number on my list of publications.

My activities over this period cover four research lines:

(a) Development and application of Wannier-based electronic-structure methods.
(b) Optical and transport responses that probe geometric properties of Bloch electrons.

(c) Weyl points (WPs) in electronic band structures.
(d) Studies of topological aspect of band theory aided by toy models.

In line (a), we developed Wannier-interpolation schemes for calculating ground-state orbital magnetization (#29), nonlinear anomalous Hall conductivity (AHC), current-induced magnetization, and natural optical activity (#43), shift photocurrent (#44), and spin-Hall conductivity (#46). In #35 we devised a method to "unfold" the k-space Berry curvature of disordered supercells, and in #38 we used it to study the valley Hall effect in disordered monolayer MoS_2. We wrote a review article on Wannier functions (#30), and a paper describing the latest release of the Wannier90 package (#36).

Main achievements in line (b):

- The formulation in #39 of a microscopic theory of intraband natural optical rotation in gyrotropic crystals in terms of the intrinsic magnetic moment of states on the Fermi surface.
- The *ab initio* study in #43 of several effects in the gyrotropic crystal trigonal tellurium:
  - Natural optical rotation, including intra- and inter-band contributions: we resolved an old controversy about the sign of the rotatory power relative to the crystal chirality.
  - Current-induced magnetization and optical rotation: we found agreement to within a factor of two with the measured change in rotatory power.
  - Nonlinear Hall effect: this was one of the first *ab initio* calculations of this effect.
  - Circular photogalvanic effect: we identified the WPs near the bottom of the conduction band as the origin of the observed sign reversal with temperature of the photocurrent.
- The development in #44 of a Wannier-interpolation scheme to calculate the shift vector, and its use in #47 to predict a large shift photocurrent response in the graphitic material BC_2N.

Work on line (c) started with a Comment (#34) on a paper that misrepresented the role of WPs below the Fermi level on the AHC in ferromagnets. In #37 we surveyed the WPs in the band structure of bcc Fe, and discovered that bcc Fe is a topological metal. In #42 we found that there exist WPs with a chiral charge of three located along a 3-fold axis in the BZ of trigonal tellurium . This could not be explained by the existing theory, according to which WPs along three-fold axes can have charges of magnitude two at most. We realized that the charge-three WPs in tellurium are protected by the combination of 3-fold symmetry with time reversal. This led us to develop a complete classification of WPs protected by screw-rotational symmetry with and without time reversal.

A major topic in line (d) has been the orbital magnetoelectric effect in insulators.

- The magnetoelectric effect gives rise to a surface AHC, and in #45 we developed a microscopic theory of that surface AHC; we found that in addition to the geometric Chern-Simons (CS) term, a non-geometric contribution is present.
- In #49 we studied the CS axion coupling in the hybrid Wannier representation, and found that its quantized value in the presence of certain symmetries can sometimes be inferred from visual inspection of the "Wannier band structure".
- In #52 we formulated the mirror Chern number in the hybrid Wannier representation, and related it to the quantized CS axion coupling in mirror-symmetric insulators.
- Finally, two works dealt with the recent topic of “higher-order topological insulators”:
  - In #50 we demonstrated that chiral hinge modes naturally emerge in 3D insulators undergoing a slow cyclic evolution that changes the CS axion angle by 2π.
  - In #51 we showed how the macroscopic corner charge in a rectangular insulating flake can be predicted from two ribbon calculations, which yield a bulk quadrupole moment and two edge polarizations. While these three quantities are individually gauge dependent, their sum is gauge invariant and equals the corner charge.

Over this period, I hosted six post-docs:

- Thomas Olsen [2014]. Now Associate Professor at the Technical University of Denmark.

- Daniel Gosálbez-Martínez [2014-2015]. Now post-doc at EPFL.
- Pablo Aguado Puente [2016]. Now post-doc at Queen's University Belfast.
- Stepan Tsirkin [2016-2018]. Now post-doc at the University of Zurich.
- Tomáš Rauch [2017-2018]. Now post-doc at the University of Jena.
- Julen Ibañez Azpiroz [2017-2021]. Now Ikerbasque researcher at the CFM.

Over this period I lectured in two Summer Schools and in one Masters program, was a member of several PhD defense committees, evaluated grant proposals, and co-organized one conference.

I was elected a Fellow of the American Physical Society in 2019. Citation:

"For developing the theory of geometric phases in electronic structure and its implementation in practical computational algorithms."

Part C. RELEVANT MERITS *(sorted by typology)*

C.1. Publications *(see instructions)*

The following ten publications are representative of my research output over the last ten years, both in terms of the topics, and of the collaborators involved. The citation counts were retrieved from the *Web of Science* on 24/11/2021, and the abstracts can be accessed by clicking on the DOI links.

1. *Gapless hinge states from adiabatic pumping of axion coupling*, Thomas Olsen, Tomáš Rauch, David Vanderbilt, and **Ivo Souza**, Phys. Rev. B **102**, 035166 (2020) (Editors' Suggestion) [5 citations].
2. *Computation of intrinsic spin Hall conductivities from first principles using maximally localized Wannier functions*, Ji Hoon Ryoo, Cheol-Hwan Park, and **Ivo Souza**, Phys. Rev. B **99**, 235113 (2019) [12 citations].
3. *Ab initio calculation of the shift photocurrent by Wannier interpolation*, Julen Ibañez-Azpiroz, Stepan S. Tsirkin, and **Ivo Souza**, Phys. Rev. B **97**, 245143 (2018) [38 citations].
4. *Gyrotropic effects in trigonal tellurium studied from first principles*, Stepan S. Tsirkin, Pablo Aguado Puente, and **Ivo Souza**, Phys. Rev. B **97**, 035158 (2018) [49 citations].
5. *Composite Weyl nodes stabilized by screw symmetry with and without time-reversal invariance*, Stepan S. Tsirkin, **Ivo Souza**, and David Vanderbilt, Phys. Rev. B **96**, 045102 (2017) (Editors' Suggestion) [42 citations].
6. *Gyrotropic magnetic effect and the magnetic moment on the Fermi surface*, Shudan Zhong, Joel E. Moore, and **Ivo Souza**, Phys. Rev. Lett. **116**, 077201 (2016) [109 citations].
7. *Valley Hall effect in disordered monolayer MoS_2 from first principles*, Thomas Olsen and **Ivo Souza**, Phys. Rev. B **92**, 125146 (2015) [19 citations].
8. *Chiral degeneracies and Fermi-surface Chern numbers in bcc Fe*, Daniel Gosálbez-Martínez, **Ivo Souza**, and David Vanderbilt, Phys. Rev. B **92**, 085138 (2015) (Editors' Suggestion) [45 citations].
9. *How disorder affects the Berry-phase anomalous Hall conductivity: A reciprocal-space analysis*, Raffaello Bianco, Raffaele Resta, and **Ivo Souza**, Phys. Rev. B **90**, 125153 (2014) [18 citations].
10. *Wannier-based calculation of the orbital magnetization in crystals*, M. G. Lopez, David Vanderbilt, T. Thonhauser, and **Ivo Souza**, Phys. Rev. B **85**, 014435 (2012) (Editors' Suggestion) [45 citations].

C.2. Conferences

1. *Probing the k-space Berry curvature and orbital moment in acentric crystals*, March Meeting of the American Physical Society, Los Angeles, March 2018 **(invited talk)**.
2. Axion magnetoelectric coupling and the surface Chern number, Workshop on Topological Phases of Matter, San Sebastián, September 2016 **(invited talk)**.
3. *Berry-phase effects for electrons in crystals*, Symposium in honor of Prof. Sir Michael Berry's 75th birthday, University of Bristol, April 2016 **(invited talk)**.
4. *Transport in broken-symmetry metals: Geometry, topology, and beyond*, Spring Meeting of the German Physical Society, Regensburg, March 2016 **(invited talk)**.
5. *Magnetoelectric coupling and surface anomalous Hall effect*, Workshop on *New Trends in Topological Insulators*, Sant Feliu de Guíxols (Spain), June 2013 **(invited talk)**.
6. *Applications of spinor Wannier functions to ferromagnetic metals and topological insulators*, CECAM workshop on *Efficient localised orbitals for large systems, strong correlations and excitations*, University of Cambridge, July 2012 **(invited talk)**.

C.3. Research grants

1. *Desarollo de los códigos Wannier90 y WannierBerri*, IKUR Grant from the Basque Department of Education targeted at High-Performance Computing, and awarded to the Materials Physics Center (MPC) Foundation. The funds allocated by the MPC Director to my group cover one post-doc for two years (2022-2023). (Note: I was not involved in the application to this grant, but I am a beneficiary.)
2. *Investigación colaborativa en tecnologías de fabricación avanzada para el control de la calidad del grafeno y la protección contra la corrosión en ambientes extremos – NG16FAB*, *Elkartek* Grant from the Basque government. Coordinated project with Andreas Berger (Nanogune) as the Principal Investigator (PI). Amount awarded to my subproject: €20,000. Funding period: 2017-2018.
3. *Theory and simulation of transport and optical phenomena in gyrotropic materials*, "Plan Nacional" Grant for "Generación de Conocimiento"(Ref. FIS2016-77188-P, University of the Basque Country). PI: Ivo Souza. Amount awarded: €80,000. Funding period: 2017-2020.
4. *Magnetoelectric couplings in solids and related phenomena*, Marie Curie "Career Integration Grant" from the European Commission (Ref. 7PM-PEOPLE-CIG13/02, University of the Basque Country). PI: Ivo Souza. Amount awarded: €100,000. Funding period: 2013-2017.
5. *Efectos magnetoeléctricos estáticos y ópticos en cristales*, "Plan Nacional" Grant for "Proyectos de Investigación Fundamental no Orientada", (Ref. MAT2012-33720, University of the Basque Country). PI: Ivo Souza. Amount awarded: €76,050. Funding period: 2013-2015.

Additionally, I have hosted post-docs funded by competitive fellowships that were awarded to them on the basis of jointly-written proposals. **Julen Ibañez-Azpiroz:** Two-year fellowship from the Materials Physics Center foundation (2017-2019), and two-year Marie Curie fellowship (2019-2021). **Tomáš Rauch:** Fellowship from the German national research foundation (DFG) (2017-2018). T**homas Olsen:** Fellowship from the Danish government for 2014.

C.4. Contracts, technological or transfer merits

I am a core developer of Wannier90, an open-source software package for postprocessing a set of Bloch functions to obtain a maximally-localized set of Wannier orbitals.