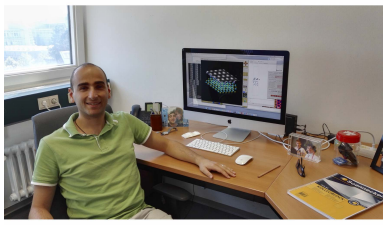
Europass Curriculum Vitae



Personal information

Name / Surname	**Prof. Di Sante Domenico**
Address	Department of Physics and Astronomy, Alma Mater Studiorum – University of Bologna, Viale C. Berti Pichat 6/2, 40127 Bologna, Italy
Personal Email	domenico.disante@unibo.it
Nationality	Italian
Date of birth	08 April 1987
Gender	Male

Employment

Dates	1 February 2021 - present
Position	**Assistant Professor (tenure track)**
Institut	Department of Physics and Astronomy, University of Bologna
Dates	1 February 2021 - present
Position	**Visiting Scholar**
Institut	Center for Computational Quantum Physics, Flatiron Institute, New York
Dates	1 December 2016 - 6 December 2020
Position	**Akademischer Rat (Academic Scientist)**
Institut	Institut für Theoretische Physik und Astrophysik, University of Würzburg
Dates	17 February 2016 - 30 November 2016
Position	**PostDOC Fellowship**
Institut	Institut für Theoretische Physik und Astrophysik, University of Würzburg
Dates	17 November 2014 - 16 February 2016
Position	**PostDOC Fellowship**
Institut	CNR-SPIN

Education

Date	May 2021
Degree	**Habilitation as Italian Professor**
Category	Full Professor in Theoretical Condensed Matter Physics (02/B2 FIS/03)

Date	April 2017
Degree	**Habilitation as Italian Professor**
Category	Associate Professor in Theoretical Condensed Matter Physics (02/B2 FIS/03)
Date	02 November 2011 - 31 October 2014
Degree	**PhD degree in Physics (15 April 2015)**
Thesis	Modeling Cross Coupling Interactions in Advanced Materials. Spin-Orbit, Multiferroicity, Disorder and Electron-Phonon Interaction.
Supervisors	Dr. Silvia Picozzi and Prof. Sergio Ciuchi
University	Department of Physical and Chemical Sciences, University of L'Aquila
Date	02 November 2011
Degree	**Admission to the PhD course in Physics**
University	Physics Department, University of L'Aquila
Date	10 October - 09 November 2011
	Fellowship with research project: "Studio teorico-computazionale dell'accoppiamento magnetoelettrico all'interfaccia Fe/$BaTiO_3$ con funzionali avanzati di scambio e correlazione"
	CNR-SPIN (Dr. S. Picozzi)
Date	01 November 2009 - 21 July 2011
Degree	**Master Degree in Physics**
University	University of L'Aquila
Final Mark	110/110 cum laude
Date	October 2006 - October 2009
Degree	**Bachelor Degree in Physics**
University	University of L'Aquila
Final Mark	110/110
Date	September 2001 - July 2006
Degree	**High-School**
School	Liceo Scientifico A. Einstein (Teramo)
Final Mark	100/100

Third-party funding

EU project 897276 (2020)	Marie Curie Global Fellowship Horizon 2020-MSCA-IF-2019, project BITMAP "aB-IniTio calculations and MAchine learning for suPerconducting collective phenomena in novel materials". Budjet: $\sim$ **270 k€**.
DFG-SFB1170 (2019-2023)	Principal Investigator (PI) of the project "Topological Fermi surface instabilities from a combined ab initio and functional renormalization group workflow". Budjet: $\sim$ **398 k€**.
DFG-SFB1170 (2019-2023)	Co-organizer of the project "i-RTG: Integrated Research Training Group", representative of young scientists. Budjet: $\sim$ **119 k€**.

Prizes and Awards

2019	Nomination in the Emerging Leaders 2020 by the JPhys Materials (IOP Publishing).
2006-2009	Student Scholarship of **12 k€** from the Italian Physics Society (SIF).
2005	Prize of the National Laboratories of GranSasso for a summer school at the Princeton University.

Research interests

Machine Learning for correlated electrons systems
Hydrodynamics of Dirac electron fluids
Topological states in 3 and 2 dimensional systems
Topological superconductivity and unconventional Fermi surface instabilities
Correlated higher-oder Dirac semimetals
Ab initio calculations of Ferroelectrics and Multiferroics
Ferroelectric Rashba Semiconductors
Electron-phonon coupling in disordered systems

Teaching

Date	Academic Year 2019/2020, Summer semester
Course	**Theory of Superconductivity**
Where	Wuerzburg University
Date	Academic Year 2019/2020, Winter semester
Course	**Computational Material Science**
Where	Wuerzburg University
Date	Academic Year 2018/2019, Summer semester
Course	**Classical Electrodynamics, Exercises**
Where	Wuerzburg University
Date	Academic Year 2018/2019, Winter semester
Course	**Computational Material Science**
Where	Wuerzburg University
Date	Academic Year 2017/2018, Summer semester
Course	**Classical Electrodynamics, Exercises**
Where	Wuerzburg University
Date	Academic Year 2017/2018, Winter semester
Course	**Computational Material Science**
Where	Wuerzburg University
Date	Academic Year 2016/2017, Summer semester
Course	**Quantum Mechanics II, Exercises**
Where	Wuerzburg University
Date	Academic Year 2016/2017, Winter semester
Course	**Computational Material Science**
Where	Wuerzburg University
Date	Academic Year 2013/2014, First semester
Course	**Teaching (Exercises): "Quantum Mechanics" and "Mathematical Methods in Physics" Courses**
Where	Department of Physical and Chemical Sciences, University of L'Aquila

Thesis Supervision

Name	Alessandro Ciavatta, University of Bologna (Bachelor thesis), 2021

Topic	Teoria della superconduttivitá e soluzione numerica dell'equazione della gap BCS
Name	Marius Fuchs, University of Wuerzburg (Master thesis), 2020
Topic	First-principles investigation of transition metal oxides thin films
Name	Schwemmer Tilman, University of Wuerzburg (Master thesis), 2019
Topic	Unconventional superconductivity in three-dimensional systems via a weak coupling renormalization group analysis
Name	Eck Philipp, University of Wuerzburg (Master thesis), 2018
Topic	Realization of a Kane-Mele-Type Quantum-Spin-Hall Insulator stabilized by Substrate Engineering
Name	Bakic Alper, University of Wuerzburg (Bachelor thesis), 2018
Topic	Realistic study of midgap states at step edges of topological crystalline insulators

Bibliometric Indicators

h-index	31 (Google Scholar)
Total Citations	3331 (Google Scholar)

Invited Talks

Date	13 April 2022
Conferene	Lectiones Amalfitanae, Amalfi Italy
Date	23 January 2020
Conferene	ECOS, Milan Italy
Date	6 September 2018
Conferene	NGSCES 2018, San Sebastian, Spain
Date	31 August 2018
Conferene	Lectiones Clitumnaliae, Campello, Italy
Date	17 March 2018
Conferene	IWEPNM 2018, Kirchberg, Austria
Date	3 March 2017
Conferene	Physics at the borderline between 1D and 2D, Bad Honnef, Germany
Date	23 and 25 June 2016
Where	CNNEM-2016, Shanghai, China
	More than 30 contributing talks and posters

Organization of Conferences

2022 Flatiron Machine Learning X Science Summer School	June 6^{th}- August 5^{th} 2022, New York, USA
NGSCES 2019	September 2^{nd}-6^{th} 2019, Pescara, Italy (https://sites.google.com/view/ngsces2019)

Refereeing

Referee for **Nature**, **Nature Communications**, **Physical Review Letters**, **Physical Review B**, **Physical Review X**, **Journal of American Chemical Society** and **New Journal of Physics**

Languages

Italian	Mother tongue
English	Good level, both written and oral
German	Basic knowledge

Full Publications List

Articles

63 D. Di Sante, M. Medvidović, A. Toschi, G. Sangiovanni, C. Franchini, A. M. Sengupta and A. J. Millis, *Deep Learning the Functional Renormalization Group*, Phys. Rev. Lett. **129**, 136402 (2022)

62 A. Troglia, C. Bigi, I. Vobornik, J. Fujii, D. Knez, R. Ciancio, G. Dražić, M. Fuchs, D. Di Sante, G. Sangiovanni, G. Rossi, P. Orgiani and G. Panaccione, *Evidence of a 2D Electron Gas in a Single-Unit-Cell of Anatase TiO_2 (001)*, Advanced Science **9**, 2105114 (2022)

61 A. Consiglio, T. Schwemmer, X. Wu, W. Hanke, T. Neupert, R. Thomale, G. Sangiovanni and D. Di Sante, *Van Hove tuning of AV_3Sb_5 kagome metals under pressure and strain*, Phys. Rev. B **105**, 165146 (2022)

60 S. Wolf, D. Di Sante, T. Schwemmer, R. Thomale and S. Rachel, *Triplet Superconductivity from Nonlocal Coulomb Repulsion in an Atomic Sn Layer Deposited onto a Si (111) Substrate*, Phys. Rev. Lett. **128**, 167002 (2022)

59 M. Kang, S. Fang, J.-K. Kim, B. R. Ortiz, S. H. Ryu, J. Kim, J. Yoo, G. Sangiovanni, D. Di Sante, B.-G. Park, C. Jozwiak, A. Bostwick, E. Rotenberg, E. Kaxiras, S. D. Wilson, J.-H. Park and R. Comin, *Twofold van Hove singularity and origin of charge order in topological kagome superconductor CsV_3Sb_5*, Nature Physics **18**, 301 (2022)

58 X. Wu, T. Schwemmer, T. Müller, A. Consiglio, G. Sangiovanni, D. Di Sante, Y. Iqbal, W. Hanke, A. P. Schnyder, M. M. Denner, M. H. Fischer, T. Neupert and R. Thomale, *Nature of Unconventional Pairing in the Kagome Superconductors $A\mathrm{V_3Sb_5}$ ($A = \mathrm{K, Rb, Cs}$)*, Phys. Rev. Lett. **127**, 177001 (2021)

57 M. Klett, T. Schwemmer, S. Wolf, X. Wu, D. Riegler, A. Dittmaier, D. Di Sante, G. Li, W. Hanke, S. Rachel and R. Thomale, *From high T_c to low T_c: Multiorbital effects in transition metal oxides*, Phys. Rev. B **104**, L100502 (2021)

56 M. Bauernfeind, J. Erhardt, P. Eck, P. K. Thakur, J. Gabel, T.-L. Lee, J. Schäfer, S. Moser, D. Di Sante, R. Claessen and G. Sangiovanni, *Design and realization of topological Dirac fermions on a triangular lattice*, Nat. Commun. **12**, 5396 (2021)

55 M. Ünzelmann, H. Bentmann, T. Figgemeier, P. Eck, J. N. Neu, F. Diekmann, S. Rohlf, J. Buck, M. Hoesch, M. Kalläne, K. Rossnagel, R. Thomale, T. Siegrist, G. Sangiovanni, D. Di Sante and F. Reinert, *Momentum-space signatures of Berry flux monopoles in a Weyl semimetal*, Nat. Commun. **12**, 3650 (2021)

55 X. Wu, K. Jiang, D. Di Sante, W. Hanke, A. P. Schnyder, J. Hu and R. Thomale, *Surface s-wave superconductivity for oxide-terminated infinite-layer nickelates*, arXiv:2008.06009

54 V. Jovic, A. Consiglio, K. E. Smith, C. Jozwiak, A. Bostwick, E. Rotenberg, D. Di Sante and S. Moser, *Momentum for Catalysis: How Surface Reactions Shape the RuO_2 Flat Surface State*, ACS Catalysis **11**, 1749 (2021)

54 D. V. Averyanov, P. Liu, I. S Sokolov, O. E. Parfenov, I. A. Karateev, D. Di Sante, C. Franchini, A. M. Tokmachev and V. G. Storchak, *Nanoscale synthesis of ionic analogues of bilayer silicene with high carrier mobility*, Journal of Materials Chemistry C **9**, 8545 (2021)

53 A. B. Odobesko, D. Di Sante, A. Kowalski, S. Wilfert, F. Friedrich, R. Thomale, G. Sangiovanni and M. Bode, *Observation of tunable single-atom Yu-Shiba-Rusinov states*, Physical Review B **102**, 1745049 (2020)

52 D. Di Sante, J. Erdmenger, M. Greiter, I. Matthaiakakis, R. Meyer, D. R. Fernandez, R. Thomale, E. van Loon, T. Wehling, *Turbulent hydrodynamics in strongly correlated Kagome metals*, Nat. Commun. **11**, 3997 (2020)

51 P Schütz, M Kamp, D Di Sante, A Lubk, B Büchner, G Sangiovanni, M Sing, R Claessen, *Electronic structure of epitaxial perovskite films in the two-dimensional limit: Role of the surface termination*, Applied Physics Letters **116**, 201601 (2020)

50 M. Ünzelmann, H. Bentmann, P. Eck, T. Kisslinger, B. Geldiyev, J. Rieger, S. Moser, R. C. Vidal, K. Kissner, L. Hammer, M A. Schneider, T. Fauster, G. Sangiovanni, D. Di Sante and F. Reinert, *Orbital-driven Rashba effect in a binary honeycomb monolayer AgTe*, Phys. Rev. Lett. **124**, 176401 (2020)

49 X. Wu, D. Di Sante, T. Schwemmer, W. Hanke, H. Y. Hwang, S. Raghu and R. Thomale, *Robust $d_{x^2-y^2}$-wave superconductivity of infinite-layer nickelates*, Phys. Rev. B **101**, 060504(R) (2020)

48 M. Fuchs, P. Liu, T. Schwemmer, G. Sangiovanni, R. Thomale, C. Franchini and D. Di Sante and S. Moser, *Kagome metal-organic frameworks as a platform for strongly correlated electrons*, Journal of Physics: Materials **3**, 025001 (2020)

47 D. M. Mahler, J.-B. Mayer, P. Leubner, L. Lunczer, D. Di Sante, G. Sangiovanni, R. Thomale, E. M. Hankiewicz, H. Buhmann, C. Gould and L. W. Molenkamp, *Interplay of Dirac nodes and Volkov-Pankratov surface states in compressively strained HgTe*, Phys. Rev. X **9**, 031034 (2019)

46 X. Wu, M. Fink, W. Hanke, R. Thomale and D. Di Sante, *Unconventional superconductivity in a doped quantum spin Hall insulator*, Phys. Rev. B **100**, 041117(R) (2019)

45 D. Di Sante, X. Wu, M. Fink, W. Hanke and R Thomale, *Triplet superconductivity in the Dirac semimetal Germanene on a substrate*, Phys. Rev. B **99**, 201106(R) (2019)

44 C.-H. Min, H. Bentmann, J. N. Neu, P. Eck, S. K. Moser, T. Figgemeier, M. Ünzelmann, K. Treiber, P. Lutz, R. Koch, C. Jozwiak, A. Bostwick, E. Rotenberg, R. Thomale, G. Sangiovanni, T. Siegrist, D. Di Sante and F. Reinert, *Orbital Fingerprint of Topological Fermi Arcs in a Weyl Semimetal*, Phys. Rev. Lett. **122**, 116402 (2019)

43 S. Ok, L. Muechler, D. Di Sante, G. Sangiovanni, R. Thomale and T. Neupert, *Custodial glide symmetry of quantum spin Hall edge modes in WTe_2 monolayer*, Phys. Rev. B **99**, 121105(R) (2019)

42 P. K. Das, D. Di Sante, F. Cilento, C. Bigi, D. Kopic, D. Soranzio, A. Sterzi, J. A. Krieger, I. Vobornik, J. Fujii, T. Okuda, V. N. Strocov, M. B. H. Breese, F. Parmigiani, G. Rossi, S. Picozzi, R. Thomale, G. Sangiovanni, R. J. Cava and G. Panaccione, *Electronic properties of candidate type-II Weyl semimetal WTe_2. A review perspective*, Electron. Struct. **1**, 014003 (2019)

41 J. Slawinska, D. Di Sante, S. Varotto, C. Rinaldi, R. Bertacco and S. Picozzi, *Fe/GeTe(111) heterostructures as an avenue towards "ferroelectric Rashba semiconductors"-based spintronics*, Phys. Rev. B **99**, 075306 (2019)

40 D. Di Sante, P. Eck, M. Bauernfeind, M. Will, R. Thomale, J. Schäfer, R. Claessen and G. Sangiovanni, *Towards Topological Quasi-Freestanding Stanene via Substrate Engineering*, Phys. Rev. B **99**, 035145 (2019)

39 S. Ciuchi, D. Di Sante, V. Dobrosavljević and S. Fratini, *The origin of Mooij correlations in disordered metals*, npj Quantum Materials **3**, 44 (2018)

38 P. K. Das, J. Slawinska, I. Vobornik, J. Fujii, A. Regoutz, J. M. Kahk, D. O. Scanlon, B. J. Morgan, C. McGuinness, E. Plekhanov, D. Di Sante, Y.-S. Huang, R.-S. Chen, G. Rossi, S. Picozzi, W. R. Branford, G. Panaccione and D. J. Payne, *Role of spin-orbit coupling in the electronic structure of IrO_2*, Phys. Rev. Materials **2**, 065001 (2018)

37 C. Rinaldi, S. Varotto, M. Asa, J. Slawinska, J. Fujii, G. Vinai, S. Cecchi, D. Di Sante, R. Calarco, I. Vobornik, G. Panaccione, S. Picozzi and Riccardo Bertacco, *Ferroelectric Control of the Spin Texture in GeTe*, Nano Lett. **18**, 2751 (2018)

36 X. Wu, H. O. Jeschke, D. Di Sante, F. O. von Rohr, R. J. Cava and R. Thomale, *Origin of the pressure-dependent T_c valley in superconducting simple cubic phosphorus*, Phys. Rev. Materials **2**, 034802 (2018)

35 J. He, D. Di Sante, R. Li, X.-Q. Chen, J. M. Rondinelli and C. Franchini, *Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide*, Nat. Commun. **9**, 492 (2018)

34 P. Schütz, D. Di Sante, L. Dudy, J. Gabel, M. Stübinger, M. Kamp, Y. Huang, M. Capone, M.-A. Husanu, V. N. Strocov, G. Sangiovanni, M. Sing and R. Claessen, *Dimensionality-Driven Metal-Insulator Transition in Spin-Orbit-Coupled $SrIrO_3$*, Phys. Rev. Lett. **119**, 256404 (2017)

33 S. Hu, H. Gao, Y. Qi, Y. Tao, Y. Li, J. R. Reimers, M. Bokdam, C. Franchini, D. Di Sante, A. Stroppa and W. Rei, *Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings*, J. Phys. Chem. C **121**, 23045 (2017)

32 D. Di Sante, A. Hausoel, P. Barone, J. M. Tomczak, G. Sangiovanni and R. Thomale, *Realizing double Dirac particles in the presence of electronic interactions*, Phys. Rev. B **96**, 121106(R) (2017)

31 D. Di Sante, P. K. Das, C. Bigi, Z. Ergönenc, N. Gürtler, J. A. Krieger, T. Schmitt, M. N. Ali, G. Rossi, R. Thomale, C. Franchini, S. Picozzi, J. Fujii, V. N. Strocov, G. Sangiovanni, I. Vobornik, R. J. Cava and G. Panaccione, *Three-Dimensional Electronic Structure of the Type-II Weyl Semimetal WTe_2*, Phys. Rev. Lett. **119**, 026403 (2017)

30 D. Di Sante, S. Fratini, V. Dobrosavljević and S. Ciuchi, *Disorder-driven metal-insulator transitions in deformable lattices*, Phys. Rev. Lett. **118**, 036602 (2017)

29 V.V. Volobuev, P.S. Mandal, M. Galicka, O. Caha, J. Sánchez-Barriga, D. Di Sante, A. Varykhalov, A. Khiar, S. Picozzi, G. Bauer, P. Kacman, R. Buczko, O. Rader and G. Springholz, *Giant Rashba Splitting in $Pb_{1-x}Sn_xTe$ (111) Topological Crystalline Insulator Films Controlled by Bi Doping in the Bulk*, Adv. Mater. **29**, 1604185 (2017)

28 P. Sessi, D. Di Sante, A. Szczerbakow, F. Glott, S. Wilfert, H. Schmidt, T. Bathon, P. Dziawa, M. Greiter, T. Neupert, G. Sangiovanni, T. Story, R. Thomale, M. Bode, *Robust spin-polarized midgap states at step edges of topological crystalline insulators*, Science **354**, 1269 (2016)

27 E. Bruyer, D. Di Sante, P. Barone, A. Stroppa, M.-H. Whangbo and S. Picozzi, *Possibility of combining ferroelectricity and Rashba-like spin splitting in monolayers of the 1T-type transition-metal dichalcogenides MX_2 (M = Mo,W; X = S,Se,Te)*, Phys. Rev. B **94**, 195402 (2016)

26 W.-P. Zhao, C. Shi, A. Stroppa, D. Di Sante, F. Cimpoesu and W. Zhang, *Lone-Pair-Electron-Driven Ionic Displacements in a Ferroelectric Metal–Organic Hybrid*, Inorg. Chem. **55**, 10337 (2016)

25 D. Di Sante, P. Barone, A. Stroppa, K. F. Garrity, D. Vanderbilt and S. Picozzi, *Intertwined Rashba, Dirac and Weyl Fermions in Hexagonal Hyperferroelectrics*, Phys. Rev. Lett. **117**, 076401 (2016)

24 A. Stroppa, P. Barone, D. Di Sante, M. Cuoco, S. Picozzi and M.-H. Whangbo, *Analogy between Jahn-Teller distortion and Rashba spin splitting, and Jahn-Teller counterpart of spin texture*, Int. J. Quantum Chem. **116**, 1442 (2016)

23 P.K. Das, D. Di Sante, I. Vobornik, J. Fujii, T. Okuda, E. Bruyer, A. Gyenis, B.E. Feldman, J. Tao, R. Ciancio, G. Rossi, M.N. Ali, S. Picozzi, A. Yadzani, G. Panaccione and R.J. Cava, *Layer-dependent quantum cooperation of electron and hole states in the anomalous semimetal WTe_2*, Nat. Commun. **7**, 11355 (2016) (Correction)

22 P.K. Das, D. Di Sante, I. Vobornik, J. Fujii, T. Okuda, E. Bruyer, A. Gyenis, B.E. Feldman, J. Tao, R. Ciancio, G. Rossi, M.N. Ali, S. Picozzi, A. Yadzani, G. Panaccione and R.J. Cava, *Layer-dependent quantum cooperation of electron and hole states in the anomalous semimetal WTe_2*, Nat. Commun. **7**, 10847 (2016)

21 M. Ptak, M. Maczka, A. Gagor, A. Sieradzki, A. Stroppa, D. Di Sante, J.M. Perez-Mato and L. Macalik, *Experimental and theoretical studies of structural phase transition in a novel polar perovskite-like $[C_2H_5NH_3][Na_{0.5}Fe_{0.5}(HCOO)_3]$ formate*, Dalton Transactions **45**, 2574 (2016)

20 M. Liebmann, C. Rinaldi, D. Di Sante, J. Kellner, C. Pauly, R.N. Wang, J.E. Boschker, A. Giussani, S. Bertoli, M. Cantoni, L. Baldrati, M. Asa, I. Vobornik, G. Panaccione, D. Marchenko, J. Sánchez-Barriga, O. Rader, R. Calarco, S. Picozzi, R. Bertacco, M. Morgenstern, *Giant Rashba-Type Spin Splitting in Ferroelectric GeTe(111)*, Adv. Mater. **28**, 560 (2016)

19 S. Ghosh, D. Di Sante and A. Stroppa, *Strain Tuning of Ferroelectric Polarization in Hybrid Organic Inorganic Perovskite Compounds*, J. Phys. Chem. Lett. **6**, 4553 (2015)

18 Y.F. Nie, D. Di Sante, S. Chatterjee, P.D.C. King, M. Uchida, S. Ciuchi, D.G. Schlom, and K.M. Shen, *Formation and Observation of a Quasi-Two-Dimensional d(xy) Electron Liquid in Epitaxially Stabilized $Sr_{2-x}La_xTiO_4$ Thin Films*, Phys. Rev. Lett. **115**, 096405 (2015)

17 Y.Liu, C.Zhang, X. Yuan, T. Lei, C. Wang, D. Di Sante, A. Narayan, L. He, S. Picozzi, S. Sanvito, R. Che and F. Xiu, *Gate-tunable quantum oscillations in ambipolar Cd_3As_2 thin films*, NPG Asia Materials **7**, e221 (2015)

16 D. Di Sante, P. Barone, E. Plekhanov, S. Ciuchi and S. Picozzi, *Robustness against Disorder of Relativistic Spectral Properties in Chalcogenide Alloys*, Sci. Rep. **5**, 11285 (2015)

15 D. Di Sante, A. Stroppa, P. Barone, M.-H. Whangbo, S., *Emergence of ferroelectricity and spin-valley properties in two-dimensional honeycomb binary compounds*, Phys. Rev. B **91**, 161401(R) (2015) (Editors' Suggestion)

14 A. Stroppa, D. Di Sante, P. Barone, M. Bokdam, G. Kresse, C. Franchini, M.-H. Whangbo and S. Picozzi, *Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskites*, Nat. Commun. **5**, 5900 (2014)

13 R. Wang, J. Boschker, E. Bruyer, D. Di Sante, S. Picozzi, K. Perumal, A. Giussani, H. Riechert and R. Calarco, *Towards Truly Single Crystalline GeTe Films: The Relevance of the Substrate Surface*, J. Phys. Chem. C **118**, 29724 (2014)

12 A. Narayan, D. Di Sante, S. Picozzi and S. Sanvito, *Topological tuning in three-dimensional Dirac semimetals*, Phys. Rev. Lett. **113**, 256403 (2014)

11 E. Plekhanov, P. Barone, D. Di Sante and S. Picozzi, *Engineering relativistic effects in ferroelectric SnTe*, Phys. Rev. B **90**, 161108(R) (2014)

10 D. Di Sante and S. Ciuchi, *Strong interplay between electron-phonon interaction and disorder in low doped systems*, Phys. Rev. B **90**, 075111 (2014)

9 P. Barone, D. Di Sante and S. Picozzi, *Improper ferroelectricity at CaTiO3 and CaMnO3 Twin Walls*, Phys. Rev. B, **89**, 144104 (2014)

8 D. Di Sante, A. Stroppa, P. Jain and S. Picozzi, *Tuning the ferroelectric polarization in a multiferroic Metal-Organic Framework*, J. Am. Chem. Soc., **135**, 18126 (2013)

7 P. Barone, D. Di Sante and S. Picozzi, *Strain engineering of topological properties in lead-salt semiconductors*, Phys. Status Solidi RRL, **7**, No. 12, 1102-1106 (2013)

6 P. Barone, T. Rauch, D. Di Sante, J. Henk, I. Mertig and S. Picozzi, *Pressure-induced topological phase transitions in rocksalt chalcogenides*, Phys. Rev. B, **88**, 045207 (2013)

5 D. Di Sante, K. Yamauchi and S. Picozzi, *Beyond Standard Local Density Approximation in the Study of Magnetoelectric Effects in Fe/$BaTiO_3$ and Co/$BaTiO_3$ Multilayers*, J. Phys.: Condens. Matter, **25**, 066001 (2013)

4 D. Di Sante, P. Barone, R. Bertacco and S. Picozzi, *Electric Control of Giant Rashba Effect in Bulk GeTe*, Adv. Mater. **25**, 3625 (2013) (Correction)

3 D. Di Sante, P. Barone, R. Bertacco and S. Picozzi, *Electric Control of Giant Rashba Effect in Bulk GeTe*, Adv. Mater. **25**, 509 (2013)

2 D. Di Sante, A. Stroppa and S. Picozzi, *Structural, electronic and ferroelectric properties of Croconic Acid crystal: a DFT study*, Phys. Chem. Chem. Phys., **14**, 14673 (2012)

1 A. Stroppa, D. Di Sante, S. Horiuchi, Y. Tokura, D. Vanderbilt and S. Picozzi, *Polar distortions in hydrogen-bonded organic ferroelectrics*, Phys. Rev. B **84**, 014101 (2011)

Books and Chapters

2 D. Di Sante, A. Stroppa, L. Z. Tan, P. Barone, A. M. Rappe and S. Picozzi *Theoretical Modeling of Organohalide Perovskites for Photovoltaic Applications. Chapter 3.2: Ferroelectricity and Spin-Orbit Coupling in Organic-Inorganic Perovskite Halides*, CRC Press, https://www.crcpress.com/Theoretical-Modeling-of-Organohalide-Perovskites-for-Photovoltaic-Applications/Giorgi-Yamashita/p/book/9781498750783

1 E. S. Tasci, A. Stroppa, D. Di Sante, G. Giovannetti, S. Picozzi and J. M. Perez-Mato, *Research Horizons of Nanosystems Structure, Properties and Interactions. Chapter 11: The How-To Guide to Computational Crystallography*, Apple Academic Press, http://www.appleacademicpress.com/title.php?id=9781926895901