Curriculum Vitae

Dr. Sunil Wilfred D'Souza

Personal data

Date of Birth: 01th December 1983

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Positions Held:

- 2014 - 2017 : Postdoctoral Fellow, Heusler Theory Group,
  Solid State Chemistry Department,
  Max Planck Institute for Chemical Physics of Solids.
  Dresden, Germany.

- 2018 – Present: Postdoctoral Researcher, Research of Advanced Materials Group, New Technologies - Research Centre, University of West Bohemia, Plzeň , Czech Republic

Research Interest:

- Density Functional theory, Greens function based Ab intio methods, Theory of magnetism.

- Ab intio calculations of ground state, electronic and transport properties of chemically disordered systems (Intermetallics), Non-collinear Spin structures (spin spirals, skyrmions).

- Calculations of finite temperature magnetism, Methods of use are based on Classical and Quantum Monte Carlo simulations, Heisenberg models, Magnetic anisotropies.

Education

- **Doctorate (Ph.D) :**
  Institute/University: UGC-DAE Consortium for Scientific Research, Devi Ahilya Vishwavidyala, Indore, India.
  Year: 2015
  Subject: Physics
  Thesis title: Photoelectron Spectroscopy and related studies on complex metal surfaces and adlayers.

- **Master of Science (M.Sc) :**
  Institute/University: Department Of studies in Physics, University of Mysore, India.
  Year: 2007
  Subject: Physics
  Percentage of marks scored: 78.45 %
  Division / grade: First Division.

- **Bachelor of Science Education (B. Sc.Ed) :**
  Institute / University: Regional Institute of Education, University of Mysore, India.
  Year: 2005
  Subjects: Physics, Chemistry, Mathematics
  Percentage of marks scored: 76.09 %
  Division / grade: First division

- **Higher Secondary School (XII Std.) :**
  Education Board: Department of pre – university education, Govt. of Karnataka, India.
  Year: 2001
  Subjects: Physics, Chemistry, Mathematics, Computer science.
  Percentage of marks scored: 84.66 %
  Division / grade: First Division..

- **High School (X Std.) :**
  Education Board: Karnataka secondary education examination board, Govt. of Karnataka, India.
  Year: 1999
  Subjects: Mathematics, Science, Social Science, Hindi, English, Kannada.
  Percentage of marks scored: 80.16 %
  Division / grade: First Division.

Fellowships and Awards

2014: Post-Doctoral research scientist fellowship from the Max Planck Society.

2009: Senior Research Fellowship sponsored by Council of Scientific and Industrial Research (CSIR), Government of India.

2007: Junior Research Fellowship sponsored by Department of Science and Technology (DST), Government of India.

2005: First Rank in the B.Sc.Ed examination, University of Mysore, India.

2005: Vemma Reddy Memorial award for best outgoing student in Physics Laboratory, Regional Institute of Education, University of Mysore, India.

2001: Recipient of the scholarship sponsored by National Council for Educational Research and Training, Regional Institute of Education , Government of India.

Research experience

May 2014 - 2017 :
Post-doctoral research scientist
Max Planck Institute for Chemical Physics of Solids
Dresden, Germany
Prof. Claudia Felser's Group

During my first postdoctoral position at Max-Planck-Institut for Chemical Physics of Solids, Dresden, Germany. My research is focused on "*Ab-initio modeling and characterization of new functional materials*", which consists of first-principle description, explanation and modeling of material characteristics resulting in the design of new materials. In this regard, my work on the materials design includes a consistent collaboration with different experimental groups mainly associated with the magnetic, transport and electron spectroscopic measurements. My basic research interests lie in the area of functional magnetic materials with a strong emphasis on the exploration of the different magnetic mechanisms appearing in the non-collinear spin structures (spin-spirals, skyrmions) with the help of DFT based Ab-inito methods and Monte-Carlo techniques. The family of ternary Heusler compounds with their rich chemical variability provides a wide platform to accomplish this task. The simple rules associated with the chemical and magnetic ordering of the Heusler compounds provides an opportunity for modeling their electronic, magnetic and transport properties, which are of utmost significance in technological applications.

My work on the effect of chemical substitution and antisite disorder on the magnetic properties of Mn excess Ni-Mn based Heuslers has provided a fundamental understanding about the relations between the crystal structure and magnetic properties of these Heusler compounds close to the martensite/austenite phase transition which plays a vital role for the state of the art magnetocaloric applications. These studies have been published in highly reputed journals [**Phys. Rev. B** 90, 220408(R) (2014), **Adv. Mater.** 28, 3321 (2016), **J. Electron Spectrosc. and Relat. Phenom.** 208, 33 (2016) and **Phys Rev. B** 93, 134102 (2016)]

I have extensively used the Spin polarized relativistic Korringa-Kohn-Rostoker (SPRKKR) Green's function methodology and the explicit methods describing disorder (coherent potential approximation, based on a Green's function technique) for contributing to the new "disorder engineering" paradigm being developed in our group. In particular, ab-initio description of the spin transport characteristics induced by the spin selective localization in tetragonal Mn_3Ga based Heusler system (**Phys Rev. B** 91, 094203 (2015)) provides a platform for the Heusler materials with strong magnetic anisotropy and high spin polarization. Another application of this paradigm, with respect to the spin-Hall effect in the half-Heusler topological insulators was carried out by the joint efforts of our and other groups (**Phys. Rev. B** 93, 195102 (2016)).

In addition, I have developed a Graphical User Interface that has provided our group with a practical possibility to efficiently combine our ab-initio SPRKKR results directly with the large-scale Monte-Carlo simulation package, ALPS (Algorithms and Libraries for Physics

Simulations). My work on Monte-Carlo simulations based on the ab-initio calculated exchange coupling parameters for a new helical Heusler antiferromagnet Pt_2MnGa (**Nat. Commun**, 7, 12671 (2016)) assisted in distinguishing the magnetic mechanisms responsible for the long range magnetic modulations, and thereby providing the exhausting explanation for all the features experimentally observed in the neutron diffraction and magnetic measurements.

June 2007 – May 2014 :
UGC-DAE Consortium for Scientific Research,
Devi Ahilya Vishwavidyala, Indore, India.
Dr. S. R. Barman's Group

My Ph.d thesis work comprises of experimental and theoretical approach for understanding the electronic structure of intermetallic compounds belonging to the family of magnetic shape memory alloys (MSMA) and spintronic materials. As far as the experimental studies are concerned, it is focused on the investigation of the Ni_2MnGa single crystal surface in a UHV (ultra high vacuum) environment by using low energy electron diffraction and photoelectron spectroscopy. Theoretical approach has been accomplished by carrying out the electronic structure calculations by using the Spin polarized relativistic Korringa-Kohn-Rostoker (SPRKKR) band structure code to study the effect of substitutional and antisite disorder on the ground state properties of MSMA's

Ni-Mn-Ga compositions that display modulated structure in the martensite phase have low twinning stress and exhibit magnetic field induced strain. The existence of modulation in Ni_2MnGa in the low tempearture phase is interesting from the view point of fundamental research. The existence and nature of modulation in Ni_2MnGa has been well established by using x-ray diffraction and neutron diffraction techniques. It is known that the stiochiometric Ni_2MnGa exhibits a incommensurate 7M modulated structure in the bulk samples. However, whether the modulation exists at the surface of the bulk single crystal is an interesting question. To answer this question, I have carried out low energy electron diffraction experiments. This experiment shows the existence of modulation on Ni_2MnGa surface in the martensite phase. The nature of modulation is found to be surface composition dependent, incommensurate for stiochiometric and commensurate for Mn-excess Ni-Mn-Ga surface. The modifications in the electronic structure of Ni_2MnGa across the austenite to premartensite and martensite transistion accompanied by modulation are quite fascinating. The temperature dependent photoemission studies of Ni_2MnGa have demonstrated the existence of charge density wave (CDW) through the appearance of a pseudogap at the Fermi level (E_F) in the premartensite phase. These results are published in [**Surf. Sci.** 606, 130 (2012) and **Phys Rev. B** 85, 085123 (2012)]

The Magnetic and electronic properties of Mn excess Ni-Mn-(Ga, In) have been studied by ab-initio calculations (SPRKKR). Substitution of excess Mn at the Ni site in Ni_2MnGa exhibits interesting magnetic properties. The excess Mn atoms cause antiferromagnetic interactions due to nearest neighbor Mn-Mn atoms, resulting in a ferrimagnetic ground state. For Mn-excess compositions, the total moment in the martensite phase is smaller compared to the austenite phase. This theoretical observation indicates that the Mn excess compositions will have higher magnetocrystalline anisotropy as compared to the Ni excess composition. For Mn_2NiGa, the lowest energy magnetic state obtained from theory by considering the antisite disorder between

Mn and Ga atoms as reported in the literature is found to be in agreement with experiments. The presence of antisite disorder indicates the existence of ferromagnetic (FM) clusters in the Mn_2NiGa ferrimagnetic matrix giving rise to a spin value like behavior. These studies have been published in [**Phys. Rev. Lett**. 109, 246601, (2012), **Phys Rev. B** 87, 144412 (2013) and **J. Phys.: Condens. Matter.** 26, 506001 (2014)]

The experimental observation of large magnetic moment (= 4.95 μB/Mn atom) with high degree of spin polarization in cubic $CeMnNi_4$ has induced interest in this class of soft ferromagnetic intermetallic compound. Due to the high degree of transport spin polarization this intermetallic compound can be of potential use for spintronic applications. Recent experiments have reported antisite disorder between Mn and Ni atoms in $CeMnNi_4$. This experimental observation served has a motivation to investigate the effect of antisite disorder on the spin polarization in this material. Hence, SPRKKR calculations were performed by considering the Mn−Ni antisite defect. We have varied the extent of disorder from 0% to 16% and found that the total spin magnetic moment decreases from 4.86 μ_B/f.u to 4.47μ_B/f.u. The calculated spin polarization for 16% antisite disorder amounts to -27%, compared to -35% for ordered (0%) CeMnNi4. This demonstrates that the presence of Mn−Ni antisite disorder reduces the spin polarization in $CeMnNi_4$. Besides, the Fermi level of both the spin channels for 0% disorder is observed to lie inside a deep pseudogap. The existence of disorder results in the filling up of the pseudogap.

Techniques/Methods used:

Computational Methods:

- Spin polarized fully relativistic Korringa-Kohn-Rostoker (SPRKKR) band structure code from Prof. Hubert's Group, LMU, Munich, Germany. This code has been used to calculate the electronic structure of ordered and disordered (substitutional and antisite) magnetic solids such as, Mn based Ferromagnetic shape memory alloys.

- Classical and Quantum Monte Carlo Simulations as implemented in the ALPS (Algorithms and Libraries for Physics Simulations) package.

Experimental Techniques:

- Photoelectron spectroscopy (XPS and ARPES)
- Low energy electron diffraction (LEED).
- Inverse photoemission spectroscopy (IPES).

List of Publications

Refereed Journal

1. P. Sadhukhan, **S. W. D′Souza**, V. K. Singh, R. S. Dhaka, A. Gloskovskii, S. K. Dhar, P. Raychaudhuri, A. Chainani, A. Chakrabarti, and S. R. Barman, Role of antisite disorder, electron-electron correlations, and a surface valence transition in the electronic structure of CeMnNi4, **Phys. Rev. B 99**, 035102 (2019).

2. P. Devi, Sanjay Singh, B. Dutta, K. Manna, **S. W. D'Souza**, Y. Ikeda, E. Suard, V. Petricek, P. Simon, P. Werner, S. Chadhov, Stuart S. P. Parkin, C. Felser, and D. Pandey, Adaptive modulation in the Ni2Mn1.4In0.6 magnetic shape-memory Heusler alloy, **Phys. Rev. B 97**, 224102 (2018).

3. Sanjay Singh, B. Dutta , **S.W. D'Souza**, M.G. Zavareh , P. Devi, A.S. Gibbs, T. Hickel, S. Chadov, C. Felser and D. Pandey, *Robust Bain distortion in the premartensite phase of a platinum-substituted Ni_2MnGa magnetic shape memory alloy*, **Nat. Commun.** 8, 1006 (2017).

4. Sanjay Singh, **S. W. D'Souza**, J. Nayak, E. Suard, L. Chapon, A. Senyshyn, V. Petricek, Y. Skourski, M. Nicklas, C. Felser and S. Chadov, *Room-temperature tetragonal non-collinear Heusler antiferromagnet Pt_2MnGa* , **Nat. Commun.** 7, 12671 (2016).

5. K. Chadova, D. Ködderitzsch, J. Minár, and H. Ebert, J. Kiss, **S. W. D'Souza**, L. Wollmann, C. Felser, S. Chadov*" Resonant impurity states in chemically disordered half-Heusler Dirac semimetals"*, **Phys. Rev. B** 93 , 195102 (2016).

6. Sanjay Singh, **S. W. D'Souza**, J. Nayak, L. Caron, E. Suard, S. Chadov and C. Felser, "*Effect of platinum substitution on the structural and magnetic properties of Ni_2MnGa ferromagnetic shape memory alloy"*, **Phys Rev. B** 93, 134102 (2016).

7. S. Singh, L. Caron, **S. W. D'Souza**,T. Fichtner, G. Porcari , S. Frabbrici, C. Shekhar , S. Chadov , M. Solzi, and C. Felser, "*Large Magnetization and Reversible Magnetocaloric Effect at the Second-Order Magnetic Transition in Heusler Materials"*, **Adv. Mater.** 28, 3321 (2016).

8. **S. W. D′Souza,** A. Chakrabarti, and S. R. Barman, "*Magnetic interactions and electronic structure of Ni–Mn–In"*, **J. Electron Spectrosc. and Relat. Phenom**. 208, 33 (2016).

9. S. Chadov, **S. W. D'Souza**, L. Wollmann, J. Kiss, G. H. Fecher, and C. Felser, "*Chemical disorder as an engineering tool for spin polarization in Mn3Ga-based Heusler systems*", **Phys Rev. B** 91, 094203 (2015).

10. M. Maniraj, **S. W. D'Souza**, Abhishek Rai, D. L. Schlagel, T. A. Lograsso, Aparna Chakrabarti, S. R. Barman*," Unoccupied electronic structure of Ni_2MnGa ferromagnetic shape memory alloy"*, **Solid State Communications**. 222, 1 (2015).

11. A. K. Nayak, C. Salazar Mejia, **S. W. D'Souza**, S. Chadov, Y. Skourski, C. Felser, and M. Nicklas, "*Large field-induced irreversibility in Ni-Mn based Heusler shape-memory alloys:A pulsed magnetic field study*", **Phys Rev. B** 90, 220408(R) (2014).
12. **S. W. D'Souza**, Tufan Roy, S. R. Barman, A. Chakrabarti, *"Magnetic properties and electronic structure of Mn–Ni–Ga magnetic shape memory alloys"*, **J. Phys.: Condens. Matter.** 26, 506001 (2014).

13. Sanjay Singh, **S. W. D'Souza**, K. Mukherjee, P. Kushwaha, S. R. Barman, S. Agarwal, P. K. Mukhopadhyay, Aparna Chakrabarti and E. V. Sampathkumaran, "*Magnetic properties and magnetocaloric effect in Pt doped Ni-Mn-Ga"*, **Appl. Phys. Lett.** 104, 231909 (2014).

14. K. R. Priolkar, P. A. Bhobe, D. N. Lobo, **S. W. D'Souza**, S. R. Barman, A. Chakrabarti, S. Emura, and T. Nakamura, *Antiferromagnetic Exchange Interactions in $Ni_2Mn_{1.4}In_{0.6}$ ferromagnetic Heusler alloy* **, Phys Rev. B** 87, 144412 (2013).

15. **S. W. D'Souza**, Abhishek Rai, J. Nayak, M. Maniraj, R. S. Dhaka, S. R. Barman, D. L. Schlagel, T. A. Lograsso and Aparna Chakrabarti, *Coexistence of charge-density wave and ferromagnetism in Ni_2MnGa,* **Phys Rev. B** 85, 085123 (2012).

16. **S. W. D'Souza**, J. Nayak, M. Maniraj, A. Rai, R. S. Dhaka, S. R. Barman, D. L. Schlagel, T. A. Lograsso, and A. Chakrabarti, *$Ni_2MnGa(100)$ ferromagnetic shape memory alloy: A surface study*, Surf. Sci. 606, 130 (2012).

17. A. Chakrabarti, **S. W. D'Souza**, and S. R. Barman, *Electronic structure of Fe_2CrSn*, **Physica B** 407, 3547 (2012).

18. Sanjay Singh, R. Rawat, S. Esakki Muthu, **S. W. D'Souza,** E. Suard, A. Senyshyn, S. Banik, P. Rajput, S. Bhardwaj, A. M. Awasthi, R. Ranjan, S. Arumugam, D. L. Schlagel, T. A. Lograsso, A. Chakrabarti, and S. R. Barman, *Spin-valve-like magnetoresistance in Mn_2NiGa at room temperature***, Phys. Rev. Lett.** 109, 246601 (2012).

19. S. Pal, S. D. Singh, S. Porwal, **S. W. D'Souza**, S. R. Barman, and S. M. Oak, *Blueshift in sulphur treated GaAsP/AlGaAs near surface quantum well*, **J. Vac. Sci. Technol. A** 30, 021401 (2012).

20. **S. W. D'Souza**, R. S. Dhaka, Abhishek Rai, M. Maniraj, J. Nayak, Sanjay Singh, D. L. Schlagel, T.A. Lograsso, Aparna Chakrabarti, and S. R. Barman, *Surface study of $Ni_2MnGa(100)$*, **Materials Science Forum** 684, 215 (2011).

21. M. Maniraj, **S. W. D'Souza**, J. Nayak, A. Rai, S. Singh, B. N. Raja Sekhar, and S. R. Barman*, High energy resolution bandpass photon detector for inverse photoemission spectroscopy***, Rev. Sci. Instrum.** 82, 093901 (2011).

22. S. Singh, M. Maniraj, **S. W. D′Souza**, R. Ranjan, and S. R. Barman, *Structural transformations in Mn_2NiGa due to residual stress*, **Appl. Phys. Lett.** 96, 081904 (2010).

23. R. S. Dhaka, A. K. Shukla, M. Maniraj, **S.W. D′Souza**, J. Nayak, and S. R. Barman, *An ultrahigh vacuum compatible sample holder for studying complex metal surfaces*, **Rev. Sci. Instrum.** 81, 043907 (2010).

24. S. Pal, S. D. Singh, S. Porwal, **S. W. D'Souza**, S. R. Barman, S. M. Oak, *Comparative study on passivation of $GaAs_{0.86}P_{0.14}/Al_{0.6}Ga_{0.4}As$ near-surface quantum well*, **J. Vac. Sci. Technol. A** 28, 1319 (2010).

25. R. S. Dhaka, **S. W. D′Souza**, M. Maniraj, A. Chakrabarti, D. L. Schlagel, T. A..Lograsso and S. R. Barman, *Photoemission study of the (100) surface of Ni_2MnGa and Mn_2NiGa ferromagnetic shape memory alloys*, **Surf. Sci.** 603, 1999 (2009).

26. A. K. Shukla, R. S. Dhaka, **S. W. D′Souza**, S. Singh, D. Wu, T. A. Lograsso, M. Krajc´i, J. Hafner, K. Horn, and S. R. Barman, *Quasiperiodic layers of free-electron metals studied using electron diffraction*, **Phys. Rev. B** 79, 134206 (2009).

27. A. K. Shukla, R. S. Dhaka, **S. W. D′Souza**, M. Maniraj, S. R. Barman, K. Horn, Ph. Ebert, K. Urban, D. Wu and T. A. Lograsso, *Manganese adlayers on i-AlPdMn quasicrystal: growth and electronic structure*, **J. Phys. Condens. Matter** 21, 405005 (2009).

Conference/School attended:

1. DPG Spring Meeting, Berlin, 15 - 20 March 2015

2. SPR-KKR Hands-On Course **,** 10 - 13 June 2012, Swiss Light Source (SLS) in the Paul Scherrer Institute (PSI) , Villigen, Switzerland.

3. Computation meets Experiment: KKR Greens functions for calculations of spectroscopic, transport and magnetic properties , 8 – 12 July 2013 at the University of Warwick, UK .

4. 55th DAE-Solid State Physics Symposium 26 - 30 December 2010 ,Manipal, India.

Talk delivered:

1. DPG Spring Meeting, Berlin, 16-03-2015, Title:"*Spin-selective electron localization induced by disorder in Mn-Co-Al Heusler alloys*".

2. Invited Talk at the Max-Planck-Institut für Eisenforschung, 09.02.2015, Title: " *Magnetic properties and electronic structure of Mn-Ni-Ga magnetic shape memory alloys*".

3. Worshop on "Magneto-elastic properties of Heusler alloys" at the Max Planck Institute for Chemical Physics of Solids, Dresden, 09.05.2014, Title:"*Magnetic Properties and electronic structure of Ni-Mn-In*".