Curriculum Vitae of

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ADDRESS FOR CORRESPONDENCE

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Old Padra Road Vadodara-391410, Gujarat, India.

EDUCATION

2017-present Pursuing Ph.D. in Physics at The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India

2016 Appointed as Junior Project Fellow in Ministry of Earth Science, Govt. of India sponsored Research Project.

2015 Master of Science (Physics), The Maharaja Sayajirao University of Baroda,

2013 Bachelor of Science (Physics, Maths, Chemistry), The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India.

2010 Higher Secondary Education (Physics, Chemistry, Botany, Zoology and Maths), Govt. Model Higher Secondary School, Vettikkavala, Kerala, India

RESEARCH INTERESTS AND EXPERIENCE

- 2D materials and high-pressure study of geological materials using Density Functional Theory.
- Computational: Familiar with Unix environment, Quantum ESPRESSO package for DFT calculations, Crystal visualization tools such as Xcrysden, VESTA and Mercury
- Experimental: Experienced in Raman spectroscopic measurements using Micro-Raman spectrometer, Collected and Analysed data of high-pressure synchrotron diffraction measurement at XPRESS beamline of Elettra.

RESEARCH VISITS

2019 Research Visit to Elettra Sinrotrone Trieste, Italy, to perform research experiment "Reinvestigation of the high pressure structural properties of three metal hydroxides viz $Ni(OH)_2$, $Co(OH)_2$ and $Mg(OH)_2$ on the XPRESS beamline of Elettra from 20th November-06th December 2019

2013 Worked as two-month project fellow on "Study of Ionosphere over Ahmedabad" at Physical Research Laboratory, Ahmedabad

AWARDS

2019 Awarded Senior Research fellowship by the Council of Scientific and Industrial Research, Ministry of HRD, Govt. of India.

2017 Received best poster award in "62nd DAE Solid State Physics Symposium organized by Bhabha Atomic Research Centre from 26-30 November 2017.

2016 Received best poster award in "6th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS 16)" held at Lucknow from 5-8 November 2016.

2016 Received best oral presentation prize in Science Conclave 2016 held at The Maharaja Sayajirao University of Baroda Vadodara

2011 Qualified National Graduate Physics Examination (NGPE) conducted by Indian Association of Physics Teachers (IAPT) within top 10% at state level.

WORKSHOPS

2021 Participated in the *All electron DFT with Fleur - a Hands-on Tutorial* held online from 12-16 April 2021

2021 Participated in the *IUCr High-Pressure Commission Workshop HPW-21* held online from 1-6 February 2021 and presented a poster introduced by an oral flash-presentation entitled "Pressure induced hydrogen order-disorder transition in metal hydroxides"

2020 Completed the three week online workshop on *Introduction to Molecular Dynamics Simulations* held during 07-24 November 2020 organised by Positron foundation, Kerala.

2018 Participated in the *Workshop on Crystal Structure Prediction: Exploring the Mendeleev Table as a Palette to Design New materials* held at the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, from 14-18 January 2019 and presented a poster

2014 Attended the workshop entitled "*DST-SERC Schoool on DFT & Beyond: Computational Materials Science and Materials Design*" held at The M. S. University of Baroda, Vadodara during 24th Nov-13th December 2014.

2013 Attended *Advanced B.Sc training program* at St. Xaviers College Ahmedabad, Gujarat India

CONFERENCES

2019 Presented a poster entitled "Lattice thermal conductivity of SiN_2, GeN_2 and SnN_2" in *64th DAE Solid State Physics Symposium (DAE SSPS 2019)* held at Indian Institute of Technology Jodhpur, Rajasthan during 18-22 December, 2019.

2019 Presented a poster entitled "High pressure phase transition in AuF_3" in the *Indus Synchrotron Users Meeting (ISUM-2019)"* held at DAVV, Indore from 27-29 March 2019

2018 Participated in *"A School on Modelling and Simulations of Materials for Energy and Environment"* held at JNCASR, Bangalore during 12-14 December 2018

2018 Presented a poster entitled "Hydrogen evolution reaction of single layer delafossite CoOOH" *in International Conference on Materials For Energy* held at S. S. Jain Subodh College, Jaipur during 6-8 December 2018

2018 Participated in *7th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS 18)"* organized by Bhabha Atomic Research Centre at DAE-Convention Centre Anushaktinagar, Mumbai during 25-29 November 2018

2018 Presented a poster entitled "Hydrogen evolution reaction of single layer delafossite CoOOH" *in National Conference on Advances in Spectroscopy: Molecules to Materials (NCASMM-2018)* held at IITRAM, Ahmedabad during 4-6 October 2018

2017 Presented a poster entitled "Strain Effect on Electronic and Lattice Dynamical Behaviour of Two Dimensional Bi BiAs and BiSb" *in 62nd DAE Solid State Physics Symposium (DAE SSPS 2017)* organized by Bhabha Atomic Research Centre during 26-30 December 2017

2017 Presented a work entitled "Hydrogen evolution reaction and electronic structure calculation of two dimensional bismuth and its alloys" in *"Recent Trends on Membranes and Separation Technology (RTMST) -2017*" at Bhavnagar during 22-23 November, 2017

2017 Presented a work entitled "Strain dependent vibrational properties of Bismuth monolayer using density functional theory", *International Conference on Spectroscopy of Biomolecules and Advanced Materials* held at Christian College, Chengannur, Kerala, India during 4-7 Oct 2017,

2016 Presented a poster entitled *"Vibrational spectra of symmetric and asymmetric δ-AlOOH under pressure: a first principles study"* in *6th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS 16)"* held at Lucknow during 5-8 November 2016

2016 Presented a poster entitled "Strain induced changes in phonon band structure of antimony monolayer using density functional theory calculations" in *61st DAE-Solid State Physics Symposium (DAE SSPS 2016)* held at KIIT University, Bhubaneswar, Odisa -during December 26-30, 2016

2016 Participated in the *Winter School on Condensed Matter Physics* held at Indian Statistical Institute, Kolkata during 11-22 January, 2016.

2015 Presented a poster entitled "First Principles Calculation of Two Dimensional Antimony And Antimony Arsenide" in *60th DAE-Solid State Physics Symposium (DAE SSPS 2019)* held at Amity University, Amity, Uttar Pradesh during December 21-25, 2015

2015 Presented a work entitled "Electronic properties of acetic acid doped graphene using First principles calculations" in an *International Conference on Application of Nanometerials in Textiles* on 23rd April 2015

PUBLICATIONS

Journals

2021 S. B. Pillai, B. Joseph, P. K. Jha, Brucite ($Mg(OH)_2$) under small perturbation: A combined first principles and synchrotron X-ray diffraction study, *J. Phys. Chem. Solids*, **154**, 110078, (2021)

2021 S. B. Pillai, D. Upadhyay, P. K. Jha, B. Joseph, A combined synchrotron diffraction and first-principles investigation on structural properties of $Co(OH)_2$ under pressure up to 7 GPa, *EPL*, **133** (1), 16002, (2021)

2021 S. B. Pillai, B. Joseph, D. Upadhyay, C. Marini, P. K. Jha, Pressure Induced Hydrogen Order–Disorder Transition in β-$Ni(OH)_2$, *J. Phys. Chem. C*, **125** (4), 2785–2792, (2021)

2020 S. B. Pillai, B. A Baraiya, D. Upadhyay, V Mankad, P. K. Jha, Catalytic activity and underlying atomic rearrangement in monolayer CoOOH towards HER and OER, *Int. J. Hydrog. Energy*, **45** (44), 23900-23907, (2020)

2020 S. B. Pillai, H. R. Soni, P. K. Jha, First principles high pressure studies on group-14 element pernitrides, *J. Alloys Compd.*, **819**, 153193, (2020)

2020 D. Kurzydłowski, A. Oleksiak, S. B. Pillai, P. K. Jha, High-pressure phase transitions of zinc difluoride up to 55 GPa, *Inorg. Chem.* **59**, 2584-2593, (2020)

2020 D. Kurzydłowski, S. Kobyakov, Z Mazej, S. B. Pillai, B Chakraborty, P. K. Jha, Unexpected persistence of cis-bridged chains in compressed AuF_3, *Chem. Commun.* **56**, 4902-4905, (2020)

2018 S. B. Pillai, S. D. Dabhi and P. K. Jha, Hydrogen evolution reaction and electronic structure calculation of two dimensional bismuth and its alloys, *Int. J. Hydrog.* Energy **43**, 21649-21654, (2018)

2018 S. B. Pillai, P. K. Jha, A. Padmalal, D. M. Maurya, and L. S. Chamyal, First principles study of hydrogen bond symmetrization in δ-AlOOH, *J. Appl. Phys* **123**, 115901, (2018)

2017 S. B. Pillai, V. Mankad and P. K. Jha, Vibrational and Raman Spectroscopic Study of Cubic Boron Nitride Under Pressure Using Density Functional Theory, *J. Electron. Mater*. **46**, 5259–5264, (2017)

Book Chapter

2019 S. B. Pillai, H. R. Soni and P. K. Jha, Strain-Induced Changes in Vibrational Properties of Arsenene and Antimonene, *Advances in Spectroscopy: Molecules to Materials*, Springer Singapore, **236**, 379-387, (2019)

Conference Proceedings

2020 S. B. Pillai, H. Soni and P. K. Jha, Lattice thermal conductivity of SiN_2, GeN_2 and SnN_2, *AIP Conf. Proc.* **2265**, 030448, (2020)

2020 D. Chodvadiya, S. B. Pillai, B Chakraborty, P. K. Jha, Strain effect on Mexican-hat dispersion and electronic band gap of 2D α-CN, *AIP Conf. Proc.* **2265**, 030377, (2020)

2018 S. B. Pillai, S. Narayan S. D. Dabhi and P. K. Jha, Strain effect on electronic and lattice dynamical behaviour of two dimensional Bi, BiAs and BiSb, *AIP Conf. Proc.* **1942**, 090022, (2018)

2017 S. B. Pillai, S. Narayan S. D. Dabhi and P. K. Jha, Strain induced changes in phonon band structure of antimony monolayer using density functional theory calculations, *AIP Conf. Proc.* **1832**, 090046, (2017)

2016 S. B. Pillai, S. Narayan, S. D. Dabhi and P. K. Jha, First principles calculation of two dimensional antimony and antimony arsenide, *AIP Conf. Proc.* **1731**, 090024, (2016)

Referees

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