

### TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type A post-doc fellowship

### [Name and surname] CURRICULUM VITAE

#### PERSONAL INFORMATION

Surname	Behera
Name	Sushant Kumar
Date of birth	[Day, month, year] 27, 06, 1992

### PRESENT OCCUPATION

Appointment		Structure
Postdoctoral Associate	Research	Materials Research Centre, Indian Institute of Science Bangalore
(August 2021-present)		

### EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
PhD	Physics	Tezpur University	2020
MSc	Physics	Tezpur University	2014
BSc	Physics	Utkal University	2012
ISc	Science	BJB Junior College	2009
Matriculation	General	R C High School	2007

### REGISTRATION IN PROFESSIONAL ASSOCIATIONS

Date registration	of	Association	City
20.01.2019		American Physical Society (student membership)	Maryland



### FOREIGN LANGUAGES

Languages	level of knowledge
English	Fluent
Italian	Basic
French	Basic

### AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award	
2020	RULA International Research Leadership Award 2020 by World	
	Research Council and United Medical Council	
2018	2018 · CSIR-NET-JRF Qualification of CSIR, Govt. of India	
2017	DST-INSPIRE SRF Fellowship Award by DST, Govt. of India	
2017	Best Innovative Technology Idea by IPR Cell, Tezpur University	
2017	International Travel Support (ITS) Award by SERB, DST, Govt. of India	
2015	INSPIRE Fellowship Award by DST, Govt. of India6	
2014	GATE Physics Qualification of MHRD, Govt. of India	
2013	Summer Research Fellowship by Indian Academy of Science	
2010	Bhavishya Jyoti Scholarship Award by Govt. of Odisha	
2009	INSPIRE Scholarship Award by DST, Govt. of India	

### TRAINING OR RESEARCH ACTIVITY

### description of activity

My field of PhD thesis work covers electronic, topological and magnetic properties of 2D materials in nanoscale. I am experienced with first principle-based DFT codes like VASP, Quantum ESPRESSO, CP2K, SIESTA, ONETEP and ATK-VNL to carry out simulations using high performing parallel cluster Computing (HPCC) facilities. Apart from this, I have solved response function properties in a van der Waals heterostructure using analytical techniques like Renormalization Group (RG) theory. Spin orbit coupling, polarization effect, effect of external electric and magnetic field on material properties, topological phase, electron transport, thermoelectric and catalytic properties for HER/OER activity, spintronics, etc. are included in my calculations. I have a strong experience in handling a few experimental instruments during my PhD work. I have authored 13 research articles of both theory experimental work in international peer reviewed journals and attended 12 international/national conferences during my PhD research work. I have experience in Python, Fortran coding along with several numerical tools (like, COSMOL, FDTD method, etc.). I am capable of executing the objectives with standard results as per my pre-knowledge in coding and data analysis.

Currently, I am studying catalytic, topological and interfacial engineering properties, emergent quantum phenomena (like, Quantum anomalous Hall (QAH) effect, and magnetic proximity effect (MPE)) of 2D vdW quantum materials using developed advanced, highly accurate and very efficient exchange-correlation density functionals (semilocal). In Parallel, I am also working currently on the electronic properties of 2D vdW heterostructures from local hybrid density functional with a special focus towards the interfacial phenomena in the nano-scale regime or supercapacitor application and energy storage. We are developing



more accurate density functional methods for solids and nano-structure systems which are cost-efficient and as accurate as exact many-body methods based on the Green function. We are also involved in the development of the methods based on adiabatic connection semilocal correlation (ACSC) and interaction strength interpolation (ISI) methods. Besides development of hybrid density functionals for solids from random phase approximation (RPA) methods to accurate description of solid properties are also my ongoing and future works.

### PROJECT ACTIVITY

Year	Project
08/2021- present	Perform research work on Emergent Phases in 2D Quantum Materials and Heterostructures
10/2020- 07/2021	Perform research work on meta-GGA level hybrid functionals in the prediction of excited state properties
08/2014- 09/2020	Perform research work on Electronic Structure, Topological effects and Magnetotransport in Two-Dimensional Materials and their heterostructures
08/2013- 06/2014	Perform master project work on Synthesis and Characterization of Ag/PPy nano composites and study its antimicrobial activity
06/2013- 07-2013	To learn and work as a summer research fellow on Synthesis and Characterization of Zirconium-Tantalum based High Temperature Functional Oxide Materials

### PATENTS

Patent		
Not Filled yet		
Not Filled yet		

### CONGRESSES AND SEMINARS

Date	Title	Place
12.08.2021	Online Poster Presentation at TYC Moire-	Imperial College, London
	August 9-13 on Magnetic Proximity Coupling	
	and Valley Symmetry Splitting in Bilayer	
	Graphene Sandwiched between	
	Ferromagnetic CrBr <sub>3</sub> system [Abstract No.	
	PP.000110]	
08.06.2021	Poster Presentation at eSSENCE-EMMC e-	Uppsala University, Sweden
	Meeting on "Multiscale modelling of	
	materials and molecules-physics-based and	
	data-driven" during June 7-8 on	
	Piezoelectric Electron-Phonon Interaction	
	in Wurtzite h-BN from Ab Initio Perturbation	
	Theory [Abstract No. VP.000210]	
05 02 2020	Online Oral Presentation at the APS March	Denver Colorado USA
05.03.2020	Meeting held at during March 2-6 on	Deriver, Colorado, USA
	Realizing the Majorana Quasiparticle	
	fermionic dynamics in (1+1) dimensional	



	Topological Quantum Materials [Abstract No. S56.00012]	
03.03.2020	Online Oral Presentation at the APS March Meeting held at during March 2-6 on Proficient quantum energy storage for <i>in- plane</i> microsupercapacitor using hybrid nanocomposite [Abstract No. U01.00010]	Denver, Colorado, USA
20.12.2019	Thesis Poster Presentation at the 64th DAE- SSPS held at during December 18-22 on Electronic, Topological and Magnetic Properties of Two-Dimensional van der Waals Quantum Systems for Potential Functionalities [Abstract No. t-0029]	Indian Institute of Technology Jodhpur, Rajasthan (India)
23.08.2019	Oral Presentation at 37th Young Physicist Colloquim held at during August 22-23 on Spin-wave mediated dynamics in two dimensional quantum van der Waals heterostructure, [Abstract No. YPC-0012]	Saha Institute of Nuclear Physics, Kolkata (India)
10.03.2019	Oral Presentation at ASM Symposium held during March 6-10 on Quantum magneto- transport behaviour and spin-wave dynamics in two dimensional van der Waals heterostructure, [Abstract No. ASM2019- 0008]	Indian Institute of Technology, Delhi (India)
06.03.2019	Oral Presentation at the APS March Meeting held during March 4-8 on Quantum spin- wave dynamics and magneto-transport behaviour in 2D van der Waals heterostructure [Abstract No. K15.00015]	Boston, Massachusetts, USA
25.04.2019	Poster Presentation at MRS Spring Meeting held during April 22-26 on Electronic, Topological and Phonon Dispersion Behaviour in vdW Layered Two-Dimensional Heterostructures [Abstract No. QN03.06.39]	Phoenix Arizona, USA
06.03.2019	Poster Presentation at ICAM Conference held at during March 6-7 on First principle understanding on electronic and magnetic behaviour in vacancy induced black Phosphorous monolayer [Abstract No. PPA84]	Jamia Milia Islamia, New Delhi (India)
07.03.2018	Oral Presentation at the APS March Meeting held during March 5-9 on Existence of non- trivial topological insulating phases in van der Waals heterostructure [Abstract No.E35.00013]	Los Angeles California, USA
20.12.2017	Poster Presentation at IWAM held during December 19-21 on Non collinear Magnetism and Phonon Dispersion Relation in Vacancy Induced Phosphorene Monolayer [Poster No. PP-160]	NIST, Brahmapur, Odisha (India)
29.08.2017	Oral Presentation at CM-Days held during August 29-31 on Electric Field Driven Non- Trivial Topological Insulating Phases in van	Department of Physics, Tezpur University, Tezpur (India)



	der Waals Heterostructure [Abstract No. 0-10]	
16.03.2017	Oral Presentation at the APS March Meeting held during March 13-17 on The role of metallic ions in nanobio hybrid catalysts from <i>ab initio</i> first principles [Abstract No. \$36.00010]	New Orleans, Louisiana, USA
13.03.2017	Poster Presentation at the APS March Meeting held during March 13-17 on Origin of minute magnetic moments in spin-orbit coupled Phosphorene monolayer [Abstract No. G1.00243]	New Orleans, Louisiana, USA
29.12.2016	Poster Presentation at the 61st DAE-SSPS held during December 26-30 on Hydrostatic Pressure Effect on Magnetic ordering in Anisotropic Co <sub>3</sub> O <sub>4</sub> Nanostructures [Abstract No. C-160]	KIIT University, Bhubaneswar, Odisha (India)
19.02.2016	Poster Presentation at MRSI Symposium held at during February 18-21 on Strain- induced structural and electronic property of graphene/h-BN vertical heterostructures: Combined Linear scaling density functional approach and molecular dynamic simulation [Abstract No. PP-75]	CSIR-NEIST, Jorhat, Assam (India)
05.12.2015	Poster Presentation at the 27th IUPAP International Conference (CCP) held during December 2-5 on Linear scaling density functional approach for realizing pressure effect on anisotropic $Co_3O_4$ nanostructures [Abstract No. MNSC-P-302]	Indian Institute of Technology, Guwahati

PUBLICATIONS

Articles (Peer Reviewed)

Renormalization group analysis of weakly interacting van der Waals Fermi system. Journal of Physics: Condensed Matter 33, 335604 (2021).

Accurate density functional made more versatile'. J. Chem. Phys. 155(2), 024103 (2021).

Improving the applicability of the Pauli kinetic energy density based semilocal functional for solids'. New Journal of Physics (2021) DOI: 10.1088/1367-2630/abfd4d.

Spin-transfer-torque mediated quantum magnetotransport in MoS<sub>2</sub>/Phosphorene vdW Heterostructure based MTJs. Physical Chemistry Chemical Physics 22(34), 19139-19146 (2020).

Proximity effects in graphene and ferromagnetic CrBr<sub>3</sub> van der Waals heterostructures. Physical Chemistry Chemical Physics 21(46), 25788-25796 (2019).

Doping nanoscale graphene domain improves magnetism in hexagonal boron nitride. Advanced Materials 31, 1805778 (2019).

Graphitic carbon nitride ornate with FeNi3 nanoparticles for flexible planar micro supercapacitor with ultrahigh energy density and quantum storage capacity. Dalton Transactions 48, 12137-12146 (2019).

Surface modified mesoporous  $g-C_3N_4@FeNi_3$  as prompt and proficient magnetic adsorbent for crude oil recovery. Applied Surface Science 473, 275-281 (2019).

PAW mediated ab initio simulations on linear response phonon dynamics of anisotropic black phosphorous monolayer for thermoelectric applications. Physical Chemistry Chemical Physics 20(41), 26688-26695 (2018).



Mechanistic Study on Electrocatalytic Hydrogen Evolution by High Efficiency Graphene/MoS2 heterostructure. Chemistry Select 2(13), 3657-3667 (2017).

Controlling the bandgap in graphene/h-BN heterostructures to realize electron mobility for high performing FETs'. RSC Advances 7(50), 31393-31400 (2017).

Driving the Electrocatalytic activity by interface electronic structure control in metalloprotein hybrid catalyst for efficient hydrogen evolution. Physical Chemistry Chemical Physics 18(33), 23220-23230 (2016).

Books/Book Chapters

Chapter 5, Two-dimensional heterostructures for potential nano electronics device applications, in 'Advances in materials design and applications', Indo American Books, ISBN 93-82661-63-8, 103-122 (2017).

### Articles in reviews

Two-Dimensional van der Waals Quantum Systems: A progressive prospect towards designing efficient nanoscale devices. (Review manuscript) Under review in Nanoscale (2021).

Band alignment heterointerface with rapid charge transfer supporting excellent photocatalytic degradation of Methylene Blue under sunlight. Under review in ACS Appl. Mater. Inter. (2021).

Improved electronic structure prediction of chalcopyrite semiconductors from a semilocal density functional with Pauli kinetic energy enhancement factor. J. Phys. Conden. Mater. (2021).

### Congress proceedings

First principle understanding on electronic and magnetic behaviour in vacancy induced black phosphorous monolayer. AIP Conf. Proc. 2276(1), 020021-1-4 (2020).

Dynamic coalescence and implosion of internal microbubbles in immobile droplet. AIP Conf. Proc. 2265(1), 030014-1-5 (2020).

Hydrostatic Pressure Effect on Magnetic ordering in Anisotropic Co3O4 Nanostructures. AIP Conf. Proc. 1832(1), 050036-1-3 (2017).

### OTHER INFORMATION

I am Sushant Kumar Behera and completed my PhD thesis entitled "Electronic, Topological and Magnetic Properties of Two-Dimensional van der Waals Quantum Systems for potential functionalities" from Advanced Functional Material Laboratory (AFML), Department of Physics, Tezpur University, India in 2020.

My field of PhD thesis work covers electronic, topological and magnetic properties of 2D materials in nanoscale. I am experienced with first principle-based DFT codes like VASP, Quantum ESPRESSO, CP2K, SIESTA, ONETEP and ATK-VNL to carry out simulations using high performing parallel cluster Computing (HPCC) facilities. Apart from this, I have solved response function properties in a van der Waals heterostructure using analytical techniques like Renormalization Group (RG) theory. Spin orbit coupling, polarization effect, effect of external electric and magnetic field on material properties, topological phase, electron transport, thermoelectric and catalytic properties for HER/OER activity, spintronics, etc. are included in my calculations. I have a strong experience in handling few experimental instruments during my PhD work. I have authored 10 research articles of both theory experimental work in international peer reviewed journals and attended 12 international/national conferences during my PhD research work. I have experience in Python, Fortran coding along with several numerical tools (like, COSMOL, FDTD method, etc.). I am capable of executing the objectives with standard results as per my pre-knowledge in coding and data analysis.

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Hall (QAH) effect, and magnetic proximity effect (MPE) of 2D vdW quantum systems using developed advanced, highly accurate and very efficient exchange-correlation density functionals (semilocal). In Parallel, I am also working currently on the electronic properties of 2D vdW heterostructures from local hybrid density functional with a special focus towards the interfacial phenomena in the nano-scale regime or supercapacitor application and energy storage. We are developing more accurate density functional methods for solids and nano-structure systems which are cost-efficient and as accurate as exact many-body methods based on the Green function. We also involve in the development of the methods based on adiabatic connection semilocal correlation (ACSC) and interaction strength interpolation (ISI) methods. Besides development of hybrid density functionals for solids from random phase approximation (RPA) methods to accurate description of solid properties are also my ongoing and future works.

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

Place and date: Bangalore, 27.08.2021

Sushart Kumar Behere

SIGNATURE

\_\_(Sushant Kumar Behera)\_