Curriculum Vitae

Dr. Ravi Kumar Trivedi, Ph.D. [N-PDF at B.A.R.C., Mumbai]
Mo. Number - 6350617212
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Publons ID - https://publons.com/researcher/1511688/ravi-trivedi
Web of Science research ID - C-1198-2018
Google Scholar link - https://scholar.google.com/citations?hl=en&user=RpT0LLMAAAAJ&view_op=list_works&sortby=pubdate
Total Citations – **183**, h-index **– 6,** i10-index **- 6**

Career Objective –

To engage in high-end research and coeducational activities using the training and knowledge received in physic and technical communication as a doctoral student in computational material science.

Editorial Board –

Member of editorial board of "International Journal of Material Science & Application" journal of Science publishing group

Reviewer –

Journals of IOP

1. Journal of Physics: Condensed matter
2. Nanotechnology
3. Material Research Express

Journals of Elsevier

1. International Journal of Hydrogen Energy
2. 2D Materials

Research Collaboration –

[Igor Mazin, Professor, George Mason University, Fairfax, Virginia, USA]

Project 1. Magnetic phase diagram of Ge doped YMn_6Sn_6 (Working on theoretical calculations), and experimental work is being led by Prof. Nirmal Ghimire, USA

[Brahmananda Chakraborty, Scientist, Bhabha Atomic Research Center, Mumbai]

Project 1. Hydrogen storage on ZTC [Zeolite Templated Carbons], doping of suitable elements using Density Functional Theory [**Under Review - PCCP**]

Project 2. Completed a review article on "Theoretical and Experimental development on defect induced ferromagnetism for spintronics application [**Under Review**]

[Prof. Debashis Bnadyopadhyay, BITS – Pilani, Pilani Campus, Rajasthan]

Project 1. UGC-SERB project work on "Substrate supported Transition metal doped alkalie earth metal clusters as Hydrogen storage elements and their applications in hydrogen fuel cells.

Research Highlights –

Book published – 1, Book-chapter – 2, Ongoing – 2 [1- Book (CRC), 1-Book Chapter]
No of published papers – 11
No of communicated paper – 4
No. of ongoing research work - 4
Total number of citation – 183, H index – 6, I-10 index - 6

PDF Experience [3 Years] –

Post-Doc [Jan. 2022-Jan. 2024] - National Post-Doc Fellow by SERB, New Delhi
[SERB file No. PDF/2021/003221]

1. Detection of different SARS Covid-19 Strains and Design of Anticancer Drug Delivery System by functionalized Carbon based Nanomaterials

Post-Doc [Dec 2018- Dec. 2021]

1. Optical absorption properties of organometallic compound [sandwich shaped]structure by using DFT

&

2. Hydrogen storage on ZTC [Zeolite Templated Carbons]

Lab- 312, Department of Physics
Indian Institute of Technology, Bombay

Post-Doc [2016-2017] Van-der Waals heterostructures – A fundamental and applications

Condensed matter and Statistical Physics lab
Department of Theoretical Physics
Institute Ruder Boskovic, Zagreb, Croatia [Europe]

Educational Qualifications -

Ph.D. [2011-2016] Study of Hybrid Semiconductor Nanoclusters and Hydrogen Storage Materials by using Density Functional Theory

Year of award – March 2017
Department of Physics, BITS – Pilani, Pilani Campus 333031, Rajasthan [India]
Examiner - Nirupam Chakraborti (IIT-Kharagpur)

M.Sc. [2006-2008] Physics with specialization in Condensed matter theory

Year of award – 2008, Percentage – 67.92
Maharaja Ganga Singh University, Bikaner, Rajasthan

B.Sc. [2003-2006] Physics, Chemistry, Math

Year of award – 2006, Percentage – 75.80
University of Bikaner, Rajasthan

Research Interest -

- 2D – Materials, Van-der Waals heterostructure, Hybrid Semiconductor Nano-clusters, Hydrogen Storage
- Clusters assembled materials, Quantum Optics

List of Publications [Book, Book chapters, Research Articles]

Books Chapters-

1. Ravi Trivedi, Brahmananda Chakraborty, Book chapter – Advances in Highly Correlated Systems, Publishers – River Publishers [**Forthcoming - ISBN: 9788770224116**]

2. Ravi Trivedi, Brahmananda Chakraborty, Design of Room temperature D^0 Ferromagnetism for Spintronic application: Theoretical Perspectives **[In press, Taylor & Francis]**

3. Ravi Trivedi, Brahmananda Chakraborty, Nanostructured Materials for Energy Storage [**Under Review, Wiley International**]

Book

1.Ravi Kumar Trivedi, Debasish Bandyopadhyay, Hybrid Nanoclusters and Applications – A Density Functional Modeling, **Lambert Academic Publisher, ISBN: 978-613-9-98674-3**

2. Ravi Trivedi, Brahmananda Chakraborty, Emerging Materials and Technologies series [**Under Process – CRC press**]

Papers –

[1] Communicated [BioMolecule Simulation]

1 **Jamelah S Al-Otaibi; Y.Sheena Mary; Y.Shyma Mary; Ravi Trivedi; Brahmananda Chakrabory; Renjith Thomas** Cluster formation between an oxadiazole derivative with metal nanoclusters (Ag/Au/Cu), graphene quantum dot sheets, SERS studies and solvent effects [**JMM, Under Review**]

[Hydrogen storage simulation]

2. Ravi Trivedi, Brahmananda Chakraborty, Hydrogen storage on Yttrium doped Zeolite templated Carbon: A density functional modeling, **IJHE** [**Under Review**]

[Hybrid nano-clusters]

1. **Ravi Trivedi, Debashis Bandyopadhyay**, Study of Electronic Structure and Stabilities of the small size EuGen (n=8-17) nanoclusters: An appraisal of (4n+2) Electronic aromaticity, **European journal of Physics Plus** [**Under Review**]

[2] Published Research Articles

1. **Jamelah S. Al-OTAIBI, Y. shyma Mary, Ravi Trivedi, Brahmananda Chakraborty Rohitash Yadav,** Molecular structure, vibrational spectra and electron localization function of biomolecules of phenothiazine derivatives and their interactions with Au and water molecule: DFT investigations in search of effective drug for SARS-Cov-2, **Journal of Biomolecular structure and Dynamics, Accepted, IF = 3.18**
2. **Ravi Trivedi**, PP Singh, Brahmananda Chakraborty Quantum Computational study of small Bismuth-Cobalt nanoalloy clusters, **Optical & Quantum Electronics**, Accepted, **IF = 2.08**
3. Debashis Bandyopadhyay, **Ravi Trivedi** Insight into catalytic behavior of TiMgn (n = 1-12) nanoclustersin hydrogen storage and dissociation process: A DFT investigation**. [International Journal of Hydrogen Energy, 2022, 47, 13418-13429, IF – 5.81]**
4. Pawel Albrycht, Jamelah S. Al-OTAIBI, Y. shyma Mary, **Ravi Trivedi**, Brahmananda Chakraborty, Surface enhanced Raman scattering investigation of pioglitazone on silver and silver-

gold metal substrates – Experimental analysis and theoretical modeling using DFT, **Journal of Molecular Structure, 2021, 1244, 13092, IF – 3.18**

5. JS Al-Otaibi, YS Mary, YS Mary, **Ravi Trivedi**, B Chakraborty, Theoretical investigation on the adsorption of melamine in Al12/B12-N12/P12 fullerene-like nanocages: a platform for ultrasensitive detection of melamine, **Chemical Papers, 2021, 1-14, IF – 2.0**
6. **Ravi Trivedi,** Debashis Bandyopadhyay**,** Study of Electronic Structure, Stabilities and Electron Localization Behavior of AgPbn (n=1-14) Nanoclusters: A First Principal Investigation, **Physica E-Low Dimensional System and Nanostructures**, **2021, 131, 114725 IF – 3.57**
7. **Ravi Trivedi,** Vikash Mishra**, E**xploring the structural stability order and electronic properties of transition metal M@Ge12 (M = Co, Pd, Tc, and Zr) doped germanium cage clusters - A density functional simulation, **Journal of Molecular Structure, Oct - 2020, 1226, 129371 IF – 3.18**
8. **Ravi Trivedi**, Debashis Bandyopadhyay, Insights of the role of shell closing model and NICS in the stability of NbGe n (n = 7-18) clusters: A first principle investigation. **Journal of Material Science, 2018, 54, 515-528, IF – 3.552**
9. **Ravi Trivedi**, Debashis Bandyopadhyay, Evolution of electronic and vibrational properties of M@X n (M= Ag, Au, X= Ge, Si, n= 10, 12, 14) clusters – A density functional modeling. **Journal of Material Science, 2018, 53, 8263-8273, IF- 3.552**
10. **Ravi Trivedi**, Debashis Bandyopadhyay, Study of adsorption and dissociation pathway of H2 molecule on Mg n Rh (n = 1-10) clusters: A first principle investigation. **International journal of Hydrogen energy, 2016, 41, 20113-20121, IF – 5.81**
11. **Ravi Trivedi**, Debashis Bandyopadhyay, Hydrogen storage in small size Mg n Co nanocluster-A density functional investigation, **International journal of Hydrogen energy, 2015, 40, 12727- 12735 IF – 5.81**
12. **Ravi Trivedi**, Kapil Dhaka, Debashis Bandyopadhyay, Study of electronic properties, stabilities and magnetic quenching of molybdenum-doped germanium clusters: A density functional investigation, **RSC advance, 2014, 4, 64825, IF – 3.10**
13. Kapil Dhaka, **Ravi Trivedi**, Debashis Bandyopadhyay, Electronic structure and stabilities of Ni- doped germanium nanoclusters: A density functional modeling study (August 2013), **J Mol Model 19: 1473-1488. IF – 1.52**

Conference paper -

- Kapil Dhaka, Ravi Trivedi, Debashis Bandyopadhyay, Magnetic behavior in Cr 2 @Ge n (n= 1-12) clusters- A density functional investigation, AIP, 2014 volume 1591, p 1498

Computational Skills -

Programming tools:	Learning PYTHON and FORTRAN
Operating System:	Linux and Windows
Software application:	La-tex, MS Office
Simulation Software:	Gaussian 03, VASP, ATK-Quantum, Quantum Espresso, LMTO code [To do research work]

Membership/Fellowship of other institutions/professional societies

10. Institute Scholarship for pursuing Ph.D. during 2011-2016
11. Project fellowship for Post-Doctoral research in IRB, Zagreb during Dec-2016 -Dec 2017
12. Certificate of Recognized reviewer from ELSEVIER.

International Visit –

1. July 3-18, 2016, International Center for Theoretical Physics, ICTP, Trieste, Italy [**Fully financial supported by ICTP, Trieste, Italy**]
2. Dec 2016-Dec 2017, Institute Ruder Boskovic, Zagreb, Croatia for pursuing Post-Doc.
3. 2019 May 11^{th} to 21^{st}, Attended 3^{rd} Questaal School at Daresbury Laboratory, **Warrington, U.K**.[**Supported by IIT – Bombay**]

Invited Lecturers –

1. Delivered a talk on "Van-der Waals Heterostructures – A fundamental and applications" in Department of Physics, **Mohan lal Sukhadiya University, Udaipur**. (13 April -2017)
2. Delivered a talk on "Van-der Waals Heterostructures – A fundamental and applications" in Department of Industrial Chemistry, **Mohan lal Sukhadiya University, Udaipur**. (15 April 2017).

Miscellaneous Information –

1Language in which I am comfortable is English and Hindi for research, teaching and working.

2. I have working experience with Gaussian 03, VASP and Quantum wise electronic structure simulation packages.

Post-Doctoral work [At present, IIT-Bombay, Dec – 2018 to Present]

1. Superconductivity in a known hydride was first reported in 1970, when Th_4H_{15} was identified to have a Tc of 8K at ambient pressure. The searching for high-temperature superconductors in hydrogen rich metal hydrides was proposed by considering that hydrogen in a high content can play a critical role in the creation of the superconductivity of the compounds. This approach was not widely adopted until Ashcroft's suggestion, who said that high pressure conditions can metallize hydrogen rich materials that are insulators at ambient pressure. Breakthroughs were achieved in SH3 and LaH10 system, which had high Tc of 200 and 250-260 K, respectively.

   Based on these work we are working on relativistic and non-relativistic effect on superconductivity by using LMTO code. [On going work]

2. **Ferrocene** is an organometallic compound with the formula $Fe(C_5H_5)_2$. The molecule consists of two cyclopentadienyl rings bound on opposite sides of a central iron atom. Ferrocene is one of the most stable organometallic compounds with a sandwich-shape structure. So we investigated the geometries of ferrocene in both the eclipsed (D_{5h}) and the staggered (D_{5d}) conformations using first-principles density functional theory (DFT). To look for optical fingerprints of dihedral angle, UV-vis absorption calculations were also performed for dihedral angles of 18°, 36°, 54°, 72°, 90°, and 108°. In order to understand the nature of low-lying spin excitations, absorption spectra were also computed for high spin states [**Done**]

Post-Doctoral work [During IRB, Zagreb (Croatia), Dec 2016 – Dec 2017]

Creation of two layer VdW materials is done by using ab initio calculation simulation package like VASP, Quantum wise which is based on density functional theory code. Such heterostructures present exciting opportunities for new physical phenomena and device concept, arising from the uniquely tunable physical properties of two dimensional vdW materials. The discovery of graphene has initiated a new approach for building heterostructures from atomically thin crystals, which are glued together by weak Van-der Waals forces (vdW).

Webpage created by us - http://tp2.irb.hr/WEB/UKF_DATABASE/NEW_WEB/

Major contribution of my research work with specific to Ph.D.-

1. Investigation of small sized hybrid TM doped germanium and silicon semiconductor nanoclusters, and cluster assembled materials to check their electronic, magnetic and optical properties. Calculations of various thermo dynamical parameter to discuss about the size depended properties like binding energy, embedding energy, second order change in energy difference, fragmentation energy, VIP (Vertical ionization potential), VEA (Vertical electron affinity). We also calculate the NICS (Nucleus independent chemical shift criteria of aromaticity) to explain the stability and DOS (Density of States) for the most stable cluster to understand the hybridization between TM atom and Ge or Si.

2. Study of transition metal doped magnesium cluster to use it as an effective hydrogen storage materials which is more practical application to solve the possible fuel problems.

Teaching Experience -

Institute	Academic Year	Post	Work role	Course
Indian Institute of Technology, Bombay	Dec.2018- Dec. 2020	TA	Tutorial, and Labs	Electrostatics, A&MP
Presidency University, Bangalore	Autum - 2018	Assistant Professor	Teaching and Labs	Engineering Physics
RNB, Global university, Bikaner	Spring - 2018	Assistant Professor	Teaching	Electrostatics, and Solid State
Birla Institute of Technology & Science, Pilani, Rajasthan	2012-2015	Lab Instructor [During my Ph.D.]	Lab [B.Tech and M.Sc.]	Practical
Poornima Group of Institutions, Jaipur	2009-2010	Assistant Professor	Teaching	Engineering Physics
Bright Career Polytechnic college, Bikaner	2008-2009	Lecturer [HOD]	Teaching	Physics

Paper and Poster presentation in Conferences –

1. Online poster presentation at 20th international workshop on computational physics and materials science: Total energy and force method, at **ICTP, Trieste Italy, SMR3554 during 23-25 Feb 2021**
2. Poster Presentation at XXth International Workshop on the Physcis of Semiconductor Devices, S.N. Bose Institute, Kolkata during 17-20th December 2019.
3. Poster presentation on " Optical absorption properties of Ferrrocene – A first principle investigation" at **Daresbury Laboratory, Warrington, United Kingdom during May 13th to 17th , 2019**
4. Poster presentation on "Hydrogen adsorption and dissociation process on MgnRh cluster - A first principle investigation" at **ICTP, Trieste Italy, SMR2874 during 4-15 July 2016.**
5. Poster Presentation on "Hydrogen adsorption and dissociation process on Co doped Mg Nanoclusters – A DFT investigation" **at ABV-IIITM Gwalior during 18-22 Oct 2015.**
6. Oral presentation on " Research Scholar day 2015, **BITS- Pilani, Pilani campus" on 15March, 2015**

7. Oral presentation on "Study of Magnetic Quenching and Aromatic nature of Mo doped germanium cluster – A density functional investigation **at IUAC New Delhi during HPC workshop on 11-13 march 2015**
8. Oral presentation on "Study of Magnetic Quenching and Aromatic nature of Mo doped germanium cluster – A density functional investigation **at IUAC New Delhi during HPC workshop on 11-13 march 2015**
9. Poster presentation in "International Conference on Current Trend in Condensed Matter Physcis" **at Institute of Physics, (CTCMP-2015), Bhubaneswar, Feb 19-22, 2015**
10. Present Oral presentation on Research Scholar day in **BITS, Pilani, Pilani campus, March 23, 2014**

Participation in Workshop –

1. Attended "Workshop and Training on current Research trends in Condensed matter- Material Science", **at BITS, Pilani, Pilani campus, March 7-8, 2014**
2. Attended "WORKSHOP ON HIGH PERFORMANCE COMPUTING, at **Inter University Accelerator Centre, New Delhi" during 5-6 May, 2014**
3. Attended "International symposium on Science of Clusters, Nanoparticles and Nanoscale Materials (SOCNAM)", **at Central university of Rajasthan and Virginia commonwealth university, USA, March 4-7, 2013**
4. Attended "International Conference and Workshop on Nanostructured Ceramics and other Nanomaterials (ICWNCN)", **at University of Delhi, March 13-16, 2012**

Personal Details –

Name – Dr. Ravi Kumar Trivedi
Father name – Shri Kanti lal Trivedi
Date of Birth – 06 July 1987
Marital status – Married
Gender - Male
Nationality - Indian
Category – Unreserved
Mobile Number – 9414503857

Address for correspondence – Near Ganpati marble, Maloo Chowk,
Nokha – 334803, Bikaner, Rajastha

References

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