

Curriculum Vitae

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Personal Details

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Languages known: Hindi, English

Nationality: Indian

Email:

Academic Qualifications:

➤ **M. Sc. (Physics):**

[First Division]

2012 - 2014

Department of Physics, Faculty of Science,
Barkatullah University Bhopal- 462026 M. P. India

➤ **B. Sc.**

[First Division]

2009 - 2012

Rajeev Gandhi College Bhopal
Affiliated to Barkatullah University Bhopal- 462026 M. P. India

➤ **12th Class (MPBSE):**

[Second Division]

2009

Saraswati Higher Secondary School,
Kareli Dist. Narsinghpur M. P.

➤ **10th Class (MPBSE):**

[First Division]

2007

Saraswati Higher Secondary School,
Kareli Dist. Narsinghpur M. P.

Teaching Experience:

- Teaching Assistant. Department of Applied Physics, The M. S. University, Baroda – 364001, Gujarat, India. Since July 2015.

Broad Subject area: Condensed Matter and Materials Physics

Specific Area of Research Interest:

Electronic structure calculations lattice dynamics and optical properties of strongly correlated systems, metal oxides and nanomaterials. High pressure studies, polymorph exploration and crystallography of inorganic compounds and minerals.

Skills and Expertise:

- ✧ Operating Systems like, CentOS, Linux,
- ✧ Simulation Packages like Quantum Espresso, VASP, Gaussian, LAMMPS ATK-VNL
- ✧ Plotting Packages like GNUplot, Xmgrace, Matlab, Scilab, Origin Pro
- ✧ Visualization Software like XCrySDen, Vesta, GaussView, VMD etc.

Paper Presented in Conference/Visit to abroad/School/Workshop

Elettra Sincrotrone Trieste Italy Visit to perform experiments (Dec 2019).

- ✚ *Phonon and Raman Scattering of Transition Metal Carbodiimides from Bulk to Monolayer* (Poster presentation) **ICOPVS 2020**, JNCSR, Bengaluru India. (Feb 2020).

- ✚ *Computational insights into the electronic and optical properties of newly predicted delafossite CuFO₂* (Poster presentation) **DAE Solid State Physics Symposium** IIT Jodhpur Rajasthan India. (Dec 2019).
- ✚ *Study of electronic properties of CuCo_{1-x}V_xO₂ using x-ray emission (XPS) and density functional theory.* (Poster Presentation) **Indus Synchrotron Users Meeting** (ISUM-2019) DAVV, Indore, (March 27-29, 2019).
- ✚ *Electronic and Optical Properties of Ferromagnetic CuCrO₂, AgCrO₂ and AuCrO₂* (Poster presentation) **DAE Solid State Physics Symposium** Guru Jambheshwar University of Science and Technology Hisar-125001 Hariyana India. (Dec 2018).
- ✚ *Electronic and vibrational properties of two dimensional NiCN₂* (Poster presentation) at **National Conference on Recent Trends in Condensed Matter Physics**, Kolkata, West Bengal, India. (31st Oct-3rd Nov 2018).
- ✚ *Structural and vibrational properties of HCoO₂ using first principles investigation.* (Poster Presentation) International Conference on **Spectroscopy of Biomolecules and Advanced Materials** Christian College, Chengannur, Kerala, 4th - 7th Oct, (2017).
- ✚ *First principles study of pressure dependent lattice dynamics of delafossite CuAlO₂ and AuAlO₂.* (Poster Presentation) International conference on **Materials for Energy and Environment**, Gwalior, 18th - 20th Nov (2016).

Publications

1. Basant Roondhe, **Deepak Upadhyay**, Narayan Som, Sharad B Pillai, Satyam Shinde, Prafulla K Jha; “Structural, Electronic and Dynamical Properties of Curium Monopnictides: Density Functional Calculations” *J. Electr. Mater.* **46**, (2017), 1842.
2. **Deepak Upadhyay**, Arun Pratap, Prafulla K. Jha “A first principles study on structural, dynamical and mechanical stability of newly predicted delafossite HCoO₂ at high pressure” *J. Raman Spectrosc.* **50** (2019) 603-613.
3. **Deepak Upadhyay**, Basant Roondhe, Arun Pratap, Prafulla K. Jha “Two-dimensional delafossite cobalt oxyhydroxide as a toxic gas sensor” *App. Surf. Sci.* **476**, (2019), 198-204.

4. Nikunj Joshi, **Deepak Upadhyay**, Ankur Pandya, Prafulla K Jha “Predicting the stable rhodium based chalcopyrites with remarkable optical properties” *J. Appl. Phys.* **126**, (2019) 235705.
5. Sharad B. Pillai, Bhumi A Baraiya, **Deepak Upadhyay**, Venu Mankad, Prafulla K Jha “Catalytic activity and underlying atomic rearrangement in monolayer CoOOH towards HER and OER” *Int. J. Hydrogen Energy* **45** (2019) 23900
6. **Deepak Upadhyay**, Nikunj Joshi, Arun Pratap, Prafulla K. Jha “Comparative ab initio study of the structural, electronic, dynamical, and optical properties of group-I based CuMO_2 ($M = \text{H, Li, Na, K, Rb}$)” *J. Appl. Phys.* **128** (2020) 155701.
7. **Deepak Upadhyay**, Nikunj Joshi, Prafulla K Jha “Two Dimensional Hexagonal GaOOH: A Promising Ultrawide Bandgap Semiconductor for Smart Optoelectronic Applications” *Chem. Phys. Lett.* **(2020)**138310
8. Urmila M. Meshiya, Pooja Y. Raval, Nikita P. Joshi, Nimish H. Vasoya, **Deepak Upadhyay**, Prafulla K. Jha, Kunal B. Modi “Probing Fano resonance, relaxor ferroelectricity, light scattering by orbital exchange-bond, orbitons by Raman spectroscopy, and their correlation with dielectric properties of pure and Fe^{3+} Substituted calcium-copper-titanate” *Vibration. Spectrosc.* **112** (2021) 103201.
9. Sharad B. Pillai, Bobby Joseph, **Deepak Upadhyay**, Carlo Marini, Prafulla K Jha “Pressure Induced Hydrogen Order–Disorder Transition in $\beta\text{-Ni}(\text{OH})_2$ ” *J. Phys. Chem. C* **125** (2021) 2785.

Full Papers in Conference Proceedings

1. **Deepak Upadhyay**, Anjali. Patel, Arun Pratap , and Prafulla K Jha “ Electronic properties and stability criteria of rhombohedral HCoO_2 ” *AIP Conf. Proc.* **1942**, (2018) 90027.
2. **Deepak Upadhyay**, Arun Pratap, Prafulla K. Jha, “Electronic and Optical Properties of Ferromagnetic CuCrO_2 , AgCrO_2 and AuCrO_2 ”, *AIP Conf. Proc.* **2115** (2019) 030516.
3. Arun Pratap, Supriya Kasyap, Sonal Prajapati, **Deepak Upadhyay** “Bio-corrosion studies of Fe-based metallic glasses” *Mat. Tod. Proc.* (2020).
4. Nikunj Joshi, **Deepak Upadhyay**, Ankur Pandya, Prafulla K Jha “Peculiar electronics and optical properties of oxychalcogenides CuRhOX ($x = \text{S, Se, Te}$): A first principles investigation” *AIP Conf. Proc.* **2265** (2020) 030357.

5. **Deepak Upadhyay**, Arun Pratap, Prafulla K. Jha “Computational insights into the electronic and optical properties of newly predicted delafossite CuFO₂” **2265** (2020) 03061.
6. Nikunj Joshi, **Deepak Upadhyay**, Ankur Pandya, Prafulla K Jha “Exploring structural, electronic, and optical properties of the bismuth based palladium chalcopyrite” *Mat. Tod. Proc.* (2020).

References

- ❖ Prof. Arun Pratap (Ph.D Supervisor)
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- ❖ Prof. Prafulla K. Jha (Ph.D Co-Supervisor)
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- ❖ Dr. Venu Mankad
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