

## Publications Related to Thesis

- **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  $\text{CuMO}_2$  ( $M = \text{H, Li, Na, K, Rb}$ )” *J. Appl. Phys.* **128** (2020) 155701.
- **Deepak Upadhyay**, Arun Pratap, Prafulla K. Jha “A first principles study on structural, dynamical and mechanical stability of newly predicted delafossite  $\text{HCoO}_2$  at high pressure” *J. Raman Spectrosc.* **50** (2019) 603-613.
- **Deepak Upadhyay**, Arun Pratap, Prafulla K. Jha “Effects of vanadium doping on the structural and electronic properties of  $\text{CuCoO}_2$ ” (*In Communication*).
- **Deepak Upadhyay**, Anjali. Patel, Arun Pratap, and Prafulla K Jha “Electronic properties and stability criteria of rhombohedral  $\text{HCoO}_2$ ” *AIP Conf. Proc.* **1942**, (2018) 90027.
- **Deepak Upadhyay**, Arun Pratap, Prafulla K. Jha, “Electronic and Optical Properties of Ferromagnetic  $\text{CuCrO}_2$ ,  $\text{AgCrO}_2$  and  $\text{AuCrO}_2$ ”, *AIP Conf. Proc.* **2115** (2019) 030516.
- **Deepak Upadhyay**, Arun Pratap, Prafulla K. Jha “Computational insights into the electronic and optical properties of newly predicted delafossite  $\text{CuFO}_2$ ” *AIP Conf. Proc.* **2265** (2020) 03061.

## Publications Not Related to Thesis

- **Deepak Upadhyay**, Nikunj Joshi, Prafulla K Jha “Two Dimensional Hexagonal  $\text{GaOOH}$ : A Promising Ultrawide Bandgap Semiconductor for Smart Optoelectronic Applications” *Chem. Phys. Lett.* (2021)138310
- Sharad B. Pillai, Bobby Joseph, **Deepak Upadhyay**, Carlo Marini, Prafulla K Jha “Pressure Induced Hydrogen Order–Disorder Transition in  $\beta\text{-Ni(OH)}_2$ ” *J. Phys. Chem. C* **125** (2021) 2785.
- 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  $\text{Fe}^{3+}$  Substituted calcium-copper-titanate” *Vibration. Spectrosc.* **112** (2021) 103201.

- 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
- **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.
- 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.
- 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.
- Arun Pratap, Supriya Kasyap, Sonal Prajapati, **Deepak Upadhyay** “Bio-corrosion studies of Fe-based metallic glasses” *Mat. Tod. Proc.* (2020).
- Nikunj Joshi, **Deepak Upadhyay**, Ankur Pandya, Prafulla K Jha “Peculiar electronics and optical properties of oxychalcogenides CuRhOX (x= S, Se, Te): A first principles investigation” *AIP Conf. Proc.* **2265** (2020) 030357.
- 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).