Abstract Book of M.Sc. Dissertation, CDP, 2018 (Vol. 2)

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Foreword

It is my pleasure to write few words about this second volume of abstract booklet. This booklet provides information regarding the research area and topics in which students are involved for their masters' dissertation at the Central Department of Physics, Tribhuvan University, Kirtipur.

This year students have improved their writing skills and the *plagiarism level* has goes down significantly. Similar to the previous year, I have spent quite a lot time for checking format of masters' dissertation as well as plagiarism level in each thesis. For now we have set 30% tolerance level when using software *plagscan*.

This year almost all dissertations are published in the various national and a few (six) International Journal.

This year we are planning to publish a booklet describing a summery with abstract of all awarded Ph.D. in physics.

Prof. Dr. Binil Aryal
Head
Central Department of Physics, Tribhuvan University, Kirtipur
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Content

A STUDY OF FAR-INFRARED LOOP AT -61^{o} LATITUDE

Abhinna Rajbanshi
(July 2018)

ABSTRACT

We studied dust color temperature and dust mass maps of a far infrared cavity found to be located at RA (J2000) = 12^{h}20^{m}55:9^{s}, DEC (J2000) = -60^{o}39'02" In addition, the distribution of Planck function along the compression and extension of the cavity is studied. This cavity is found to have following properties: (a) it is located nearby a far infrared loop named G299+02, (b) the flux density is found to be three-fold less than that of its ambient interstellar medium surroundings, (c) it is close to the Galactic plane therefore the radiation field is strong and (d) the diameter of the cavity is greater than 0.5 degree on IRAS, The dust color temperatures are found to be in the range 23.48 K to 24:34 K. In this cavity, Planck function is found to be non-uniform along its extension and compression, suggesting the dust and grains are not in the local thermodynamical equilibrium, possibly because of external cause. It is therefore, a deviation from the Gaussian distribution is noticed in the histogram of dust color temperature. We conclude that the cavity is formed due to the high pressure events occurred in the past (e.g., AGB wind, supernova explosion).

Supervisor: Prof. Dr. Binil Aryal

AIR POLLUTION DISPERSION MODELING AND AIR POLLUTION AIRSHED MAP OF HETAUDA CEMENT INDUSTRY LTD

Anil Kumar Khadka
(July 2018)

ABSTRACT

This thesis investigates the pre-monsoon time meteorological flow characteristics and tracers (pollutant) dispersion pattern emitted from Hetauda Cement Factory. The primary aim of this study is to define the air pollution climatology of Hetauda valley and to prepare the air pollution air shed map to identify the potentially affected areas. Spatial and temporal characteristics of the prevailing meteorology have been studied using Weather Research and Forecasting (WRF) model and the tracer dispersion phenomenon have been studied using Chemical Transport Model (CTM). Spatial and temporal variation of meteorological parameters such as wind speed, wind direction and near surface temperature for the height 30 m above the ground level have been studied. Based on WRF simulations of meteorological fields, the study showed that easterly/southeasterly flow dominate the valley with wind speed ranging up to 14m/s. During the day, strong wind flows towards the western and northwestern part of valley, however the flow essentially remains same above the central valley floor throughout the day. The maximum and minimum temperature of the central valley appears to be 26 and 14 ◦C. The prolong surface inversion from early evening to late morning of next day appears to accumulate tracers within the lower breathable atmosphere. Though, the daytime mixing layer develops upto more than 2 kilometer above the ground level, the strong westward and northwestward flow appears to disperse and dilute the tracers released from the factory. The dispersion simulation showed that tracers released from factory get stagnated within the shallow surface layer from early evening to late morning of next day. The tracer concentration appears to be more than 5 ppb up to about 5 kilometer windward direction during this time. During the daytime, the concentration appears to reduce with high concentration of tracer confined within 1 kilometer windward direction. The valley disperses the tracers released towards the western/northwestern regions affecting the air quality of those areas.

Supervisor: Prof. Dr. Ram Prasad Regmi

METEOROLOGICAL AND AIR POLLUTION DISPERSION MODELING OF CHAUDHARY GROUP CEMENT INDUSTRIY, NAWALPARASI, NEPAL

Antim Sinjali
(August 2018)

ABSTRACT

Present study examined the late wintertime meteorological and air pollution transport characteristics in and around one of the largest cement industry (CGCI) located in the inner valley of western Nepal Himalaya. The meteorological fields and the air pollution transport were numerically simulated using the comprehensive Weather Research and Forecasting (WRF) and a chemical transport model (CTM) during the period of late-winter time. The areas in and around the CGCI remains relatively windy most of the time but the immediate atmosphere of the area appears to be highly stratified except during the late morning to early afternoon. Vertical dispersion of pollutants are suppressed by the prevailing meteorological situation and the only effective air pollution transport process appears to be the horizontal transport that mostly occurs towards the east/southeastern areas from late afternoon until late morning. Beyond the later morning and until late afternoon, the pollutants released at CGCI are transported towards the south/southwest. During the late afternoon and early evening, the pollutants transported towards the west crossing the Daunne mountains range. The areas like Bardaghat, Dhutibari, western part of Chitwan National Park, the areas from Dumkibas to Bharatpur including the Sunawal, Ramgram, Parashi and even Bhairahwa and Lumbini areas comes under the air pollution airshed of CGCI. Increasing number of mega cement industries over the Dumkibaas Sardi areas can have significant impacts on the prevailing ecosystem and human health including the reduced agricultural productivity and disruption in the conservation efforts in Chitwan National Park if effective emission control measures are not observed. .

Supervisor: Prof. Dr. Ram Prasad Regmi

ELECTRONIC AND MAGNETIC PROPERTIES OF ZINC DOPED PHOSPHORENE

Arjun Ghimire
(July 2018)

ABSTRACT

We have performed First-Principles calculations to study the electronic and magnetic properties of pristine as well as zinc doped phosphorene monolayer. The calculations are based on Density functional Theory (DFT) with van der Waals (vdW) interactions in DFT-D2 approach within Generalized Gradient Approximation (GGA). These calculations are carried out by using Quantum ESPRESSO (QE) software package. We have constructed unit cell of phosphorene monolayer containing four phosphorous atoms and taken 3x3 supercell for our calculations. Optimized lattice parameters of phosphorene monolayer are found to be a = 4.55 A, b = 3.31 A along X- and Y-directions and interlayer spacing is taken to be 20 A. Our study showed that phosphorene monolayer is semiconductor with direct band gap of 0.87 eV at the symmetric point T. The symmetric nature of DOS for spin-up and spin-down electrons indicates non magnetic nature of phosphorene monolayer. We found 2.78% zinc doped phosphorene is thermodynamically unstable with formation energy 3.16 eV. The 2.78% zinc doped system is direct band gap semiconductor with band gap of 0.82 eV. The Fermi level is shifted downwards indicating of hole doping. The DOS of spin-up and spin-down electrons are not symmetrical which indicates the magnetic nature of zinc doped phsophorene monolayer and magnetic moment is found to be 0.11 B per cell. The arise in magnetism is due to the structural modification of the phosphorene monolayer after doping.

Supervisor: Prof. Dr. Narayan Pd Adhikari

A STUDY OF PLANCK FUNCTION DISTRIBUTION IN THE FAR INFRARED LOOP G067+00

Ashwin Thapa Magar
(July, 2018)

ABSTRACT

A systematic search of isolated loop like structure in the far infrared (100 μm and 60 μm) IRAS (Infrared Astronomical Satellite) survey was performed using Sky View Observatory (http://skyview.gsfc.nasa.gov/). In order to find the possible candidate of isolated structure not yet studied, we used SIMBAD (http://simbad.ustrasbg.fr) database to locate discrete sources in the region. A new isolated far infrared loop like structure G067+00 (size 0.7^{o} x 0.6^{o} at galactic longitude 67.1^{o} and galactic latitude 0.4^{o} was found. In this work, we have calculated dust mass, dust color temperature, and studied the distribution of Planck's function along the extension and compression of the cavity. We also studied the flux density variation using software ALADINV2.5. The maximum and minimum dust color temperature of our region of cavity is found to be 21.73±0.16K and 23.26±0.22K. The offset value for temperature is found to be < 2K. Therefore our cavity is stable cavity. Along the major and minor diameter the distribution of Planck's function is not uniformly distributed. A deviation from second order polynomial suggest that the dusts and grains are not in the thermal equilibrium along the major and minor diameter ot the cavity. We conclude that the effect of wind (AGB wind etc.) might be responsible for this fluctuation.

Supervisor: Prof. Dr. Binil Aryal

FIRST-PRINCIPLES STUDY OF THERMOELECTRIC PROPERTIES OF BROMINE FILLED M_4Sb_{12} (M=Co,Pd)

Bibash Sapkota
(May 2018)

ABSTRACT

First-principles calculations have been performed within Density Functional Theory (DFT) and Boltzmann Transport Equations (BTE) with the help of *WIEN2k* and *BoltzTraP* package to study the electronic and transport properties of Br filled M_4Sb_{12} (M=Co, Pd). We have used Generalized Gradient Approximation (GGA) with PBE exchange correlation functional for DFT calculations. We have employed constant relaxation time approximation and rigid band approach while solving Boltzmann Transport Equations. Murnaghan Equation of State have been used to perform volume optimization of the species. For SCF calculations, 15000 k-points and for DOS calculation 25000 k-points are sampled in the first Brillion zone. Density of States and Band Structure are calculated by using modified tetrahedron method as discussed by Blochl et al. Optimized value of lattice parameter are 9:12, 9:16, 9:58 and 9:57 Å for Co_4Sb_{12}, $BrCo_4Sb_{12}$, Pd_4Sb_{12} and Pd_4Sb_{12}, respectively. Bulk modulus are 85:98, 88:36, 73:70, 77:82 GPa for Co_4Sb_{12}, $BrCo_4Sb_{12}$, Pd_4Sb_{12} and Pd_4Sb_{12}, respectively. Values of lattice parameter and bulk modulus for Co_4Sb_{12} agree reasonably with the existing researches. Study of density of states (DOS) and band structure reveals that Co_4Sb_{12} has semiconductor character with the band gap 0:15 eV while $BrCo_4Sb_{12}$, Pd_4Sb_{12} and $BrPd_4Sb_{12}$ have metallic character. Bromine acts as an acceptor when filled in Co_4Sb12 and as a donor in Pd_4Sb_{12}. At Fermi level, maximum value of $S^2\sigma_T/\kappa_c$ were found to be 0:42 (at T = 260 K), 0:38 (at T = 1000 K), 0:10 (at T = 1000 K) and 0:04 (at T = 1000 K) for Co_4Sb_{12}, $BrCo_4Sb_{12}$, $BrPd_4Sb_{12}$ and Pd_4Sb_{12}, respectively. Among the studied four species, by comparing the maximum value of $S^2\sigma_T/\kappa_c$ at different chemical potential at T = 600 K, the compounds can be arranged in the decreasing order of their thermoelectric efficiency (η) as η(Co4Sb12) > η(BrCo4Sb12) > η(Pd4Sb12) = η(BrPd4Sb12).

Supervisor: Prof. Dr. Narayan Prasad Adhikari

HYDROPHOBICITY OF SMALL ALKANE MOLECULES (PROPANE DIMER) IN SOLVENTS: A CLASSICAL MOLECULAR DYNAMICS STUDY

Bikash Panthi
(June 2018)

ABSTRACT

Molecular Dynamics (MD) simulations were performed for propane dimer in three different solvents (Water, Acetonitrile and Methanol) using GROMACS-Groningen Machine for Chemical Simulations. Hydrophobic interactions have been studied in terms of Potential of Mean Force (PMF). A series of Umbrella sampling MD simulations were carried out in each solvent separately and PMFs were calculated by using Weighted Histogram Analysis Method. Results of our study show that two minima (contact minima and solvent separated minima) characterize the PMF of propane dimer in solvent environment of water, acetonitrile and methanol. The first minima (contact minima) is deeper and was obtained at 0.49 nm, 0.50 nm and 0.53 nm for water, acetonitrile and methanol respectively. Varying the solvent environment does not seem to have much effect in the position of contact minima. However, the variation in solvent environment has shown appreciable effect in the position of second minima (solvent separated minima). The solvent separated minima was obtained at 0.84 nm, 0.90 nm and 0.96 nm for water, acetonitrile and methanol respectively. Our study reveals that the interactions between propane dimer are softer in methanol and acetonitrile than in water. The presence of competitive methyl group in acetonitrile and methanol is considered to be responsible for the softer interactions in these mediums.

Supervisor: Dr. Nurapati Pantha

STUDY OF HYDROGEN BOND EFFECT ON THE –C=O GROUP IN QUINONE MOLECULES

Binod Joshi
(July 2018)

ABSTRACT

The present work enumerates detailed computational investigation into the vibrational properties of three different quinone families, separately and comparatively in aqueous phase, which are 2-methyl-3-phytyl-1,4-naphthoquinone (phylloquinone), ubiquinone and plastoquinone. By changing the dihedral angle made by the three atoms of water molecule and the oxygen atom at the α-carbon site, we observed that the quinone species have the most stable configuration around 180 and that their energy curve follows a potential well like path, albeit with some variations. It was also observed that UQ has the lowest energy and hence, the most stable geometry. In addition to calculating energy values, we optimized the quinone configurations for frequencies and compared vibrational properties of all three molecules by placing the water molecule near the C1 and C4 oxygen atoms. Furthermore, for UQ-PQ and PhQ-PQ, we studied comparative spectra calculated in aqueous phase. The calculations for energy was undertaken using the B3LYP functional and the 6-31G+(d) basis set while the frequencies were calculated using Hartree-Fock functional of the same basis set.

Supervisor: Dr. Hari Prasad Lamichhane

ADSORPTION FREE ENERGY OF BIPHENYL AND ANILINE ON THE SURFACE OF GRAPHENE AT DIFFERENT TEMPERATURES

Binod Prasad Bhatta
(Feb 2019)

ABSTRACT

Molecular Dynamics (MD) simulations were performed for biphenyl-graphene and an aniline-graphene system in a TIP3P water model as solvent using NAMD (Nanoscale Molecular Dynamics) for simulations and VMD (Visual Molecular Dynamics) for molecular visualization, modeling and analyzing the system. The work has been accomplished at different temperatures; 250 K, 260 K, 280 K, 300 K, 320 K, and 340 K for biphenyl-graphene and 250 K, 260 K, 280 K, 300 K, 320 K, and 350 K for an aniline-graphene system at 1.03 x 10^5 Pascal. Adsorption Free-energy calculations is a classical molecular dynamics simulations which these days are utilized in a wide scope of research zones including solvation thermodynamics, molecular identification, and protein folding. In our present work, we have determined the ability of graphene to predict adsorption free energy for biphenyl and aniline using Adaptive Biasing Force (ABF) method. The adsorption free energy of both systems have been determined in the NPT ensemble in above-mentioned temperatures and found to increases slightly with an increase in temperature. The value of free energy thus calculated have been found to agree very good with the previous result with a small discrepancy of 2.13 % at 300 K for a biphenyl-graphene system.

Supervisor: Dr. Gopi Chandra Kaphle

FIRST-PRINCIPLES STUDY OF THERMOELECTRIC PROPERTIES OF CALCIUM (Ca) FILLED SKUTTERUDITE Ir_4Sb_{12}

Bipin Bhattarai
(September 2018)

ABSTRACT

First-principles calculations to study thermal and electrical properties of pristine and impurity (calcium) doped skutterudite Ir_4Sb_{12} has been carried out. Density of States (DOS) and band-structure calculations are based on Density Functional Theory (DFT) within Generalized Gradient Approximation (GGA). Transport properties like, electrical conductivity, thermal conductivity and Seebeck coefficient calculations are based on Boltzmann Transport Equations (BTE) within constant Relaxation Time Approximation (RTA). We have used WIEN2k for band-structure and DOS calculations. Transport properties are calculated using BoltzTrap software package. Volume optimization is carried out on the basis of Murnaghan equation of states. The optimized lattice parameter of pristine Ir_4Sb_{12} is found to be 9.4243 Å and that of calcium filled Ir_4Sb_{12} is 9.4949 Å. The value of lattice constant of Ir_4Sb_{12} is compared with experimental value which is within 1.89% of the experimental value. Bulk modulus of Ir_4Sb_{12} is also compared with experimental value and found to be within 11% difference. Comparison of band structure with previous calculations shows good agreement with our calculation. Our calculation showed that Ir4Sb12 is a p-type semiconductor with a narrow PBE-GGA band gap of 0.25 eV. After filling calcium, the band gap is reduced to zero showing the metallic behavior of filled compound. Filling of calcium resulted in the increase of n-type of electric conduction thereby changing p-type compound to n-type. Electronic band structure, Density of states, variations of electrical conductivity and thermal conductivity with temperature, Seebeck coefficient, constancy of the term $\kappa_c/\sigma T$; all show the calcium filled Ir_4Sb_{12} has a metallic character. At Fermi level, the maximum value of $S^2\sigma T/\kappa_c$ is found to be 0.5 for unfilled compound at temperature of 400K. Filling of calcium resulted in decrease of the value of quantity $S^2\sigma_T/\kappa_c$ which is found around 0.1 at a temperature of 1000K.

Supervisor: Prof. Dr. Narayan Pd Adhikari

TRANSPORT PROPERTIES OF VALINE IN WATER AT DIFFERENT TEMPERATURES

Deepak Pandey
(July 2018)

ABSTRACT

Molecular Dynamics simulations of Valine in water and their binary mixtures (N_{Val} = 0.003 & N_{water} = 0.997, N representing the mole fraction) have been accomplished at temperatures 293K, 303K, 313K, 323K, and 333K using the OPLS/AA force field parameters and comparing with data available in the literature. The work has been carried out using GROMACS. The OW-OW, H19-OW, N6-OW and C1/C3-OW radial distribution functions (RDFs) have been estimated. And co-ordination numbers are also determined by the self-coded FORTRAN. The self-diffusion coefficients of Valine and water have been determined by means of mean-square displacement (MSD) using Einstein's relation. The mutual diffusion coefficients of the binary mixtures have been determined using Darken's relation. The values of the diffusion coefficients have been found to agree very good with the experimental results. The temperature dependence of the diffusion coefficients have been analyzed and the analysis showed that they follow Arrhenius behavior..

Supervisor: Prof. Dr. Narayan Pd Adhikari

CO-OPERATIVE EFFECT OF ELECTRON CORRELATION AND SPIN-ORBIT COUPLING ON DOUBLE PEROVSKITES $SrLaBB'0O_6$ (B=Ni,Fe; B'=Os,Ru)

Dinesh Kumar Yadav
(Feb 2019)

ABSTRACT

We found newly synthesized double perovskite materials with transition elements consisting of 4d and 5d states that are strongly influenced by spin-orbit coupling (SOC). We investigate the electronic and magnetic properties of these newly synthesized materials $SrLaBB0O_6$ (B=Ni, Fe; B'=Os, Ru) on the basis of density functional theory. The strong electron-correlation effects (U) were considered for the B and B0-sites. We found the antiferromagnetic ground state for $SrLaNiOsO_6$, $SrLaFeOsO_6$ and $SrLaNiRuO_6$ with their easy axis along the [001]-direction. Electronic behaviors in these compounds are found to be insulating. Upon inclusion of SOC in Os-5d site leads to the opening of the very small band gap (0.03 eV) which dictates the significant influence of SOC in $SrLaFeOsO_6$. $SrLaNiOsO_6$ and $SrLaNiRuO_6$ also shows Mott-insulating behavior with band gap of 0.33 eV and 0.58 eV respectively with dominant contributions from Os-5d and Ru-4d bands around the Fermi level. Our result agrees fairly with the experimental finding for these systems. Charge ordering is found to be prominent in these compounds.

Supervisor: Dr. Gopi Chandra Kaphle

TRANSPORT PROPERTIES OF GAMMA-AMINOBUTYRIC ACID IN WATER

Esha Mishra
(June 2018)

ABSTRACT

We have carried out molecular dynamics study of diffusion of Gamma-Aminobutyric acid in water at different temperatures (298.2 K, 303.2 K, 313.2 K, 323.2 K, 333.2 K) using GROMACS- Groningen Machine for Chemical Simulations. The solute and solvent is modeled using OPLS-AA platform. The structure of the system is analyzed using RDF of different atom/molecule pairs. In all the cases, at least two or more peaks were obtained which suggests appreciable amount of interaction between atoms and molecules. The self diffusion coefficient of GABA and water is calculated from mean square displacement (MSD) plot using Einstein's relation. Binary diffusion coefficient is obtained from self diffusion coefficient using Darken's relation. Binary diffusion coefficients are found to be in good agreement with the previously reported experimental data. The temperature dependency of diffusion coefficient is found to follow Arrhenius formula..

Supervisor: Prof. Dr. Narayan Pd Adhikari

REFLECTION AND TRANSMISSION COEFFICIENTS OF ELECTROMAGNETIC WAVE EQUATION IN SCHWARZSCHILD BLACK HOLE

Gopal Neupane
(June 2018)

ABSTRACT

The electromagnetic perturbation to the Schwarzschild metric is studied. The perturbation of the Schwarzschild black hole is described by the general time-dependent Regge-Wheeler equation. We transform this equation to usual Schwarzschild coordinates. In this case, it is possible to separate a harmonic time-dependence. Then, the resulting radial equation belongs to the class of confluent Heun equation consisting of effective potential. The potential behaves like 1-D potential barrier in elementary quantum mechanics which is used to calculate the reflection and transmission coefficients near the Schwarzschild space-time using black hole boundary condition and the properties of confluent Heun function.

Supervisor: Prof. Dr. Udayaraj Khanal

ELECTRONIC AND MAGNETIC PROPERTIES OF MOLECULAR NITROGEN ADSORBED PHOSPHORENE

Govinda Kharal
(June 2018)

ABSTRACT

In the present work, we have carried out First-Principles calculations to study electronic as well as magnetic properties of pristine and nitrogen molecule adsorbed phosphorene monolayer. All these calculations were based on Density Functional Theory (DFT) along with DFT-D2 approach within Generalized Gradient Approximation (GGA). We have used Quantum ESPRESSO (QE) software package for the simulation. We expanded orthogonal unit cell of phosphorene with four phosphorus atoms per unit cell to 3 x 3 supercell of phosphorene monolayer for our calculation. Optimization of orthogonal lattice parameters of phosphorene monolayer yielded a = 4.55 Å, b = 3.31 Å along X and Y directions within 1 % error from that of experimental values. Our study show that pure phosphorene monolayer is semiconductor with direct band gap, Eg, of 0.87 eV at the symmetric point τ. Our further investigations show that adsorption of nitrogen molecule decreases band gap by negligibly small amount preserving the direct nature of energy gap. Moreover, we found the molecular nitrogen adsorption on pristine phosphorene does not change its non magnetic behavior.

Supervisor: Prof. Dr. Narayan Pd Adhikari

DUST COLOR TEMPERATURE DISTRIBUTION IN THE FAR INFRARED CAVITY NEARBY KK-LOOP G172+01

Harilal Bhattarai
(July 2018)

ABSTRACT

We studied distribution of dust color temperature and dust mass of a far infrared cavity found to be located at R.A.(J2000) = $5^h31^m33{:}3^s$ and Dec.(J2000) = $55^o41'43"$. In addition, the distribution of Planck's function along the compression and extension of the cavity is studied. This cavity is found to have following properties: (a) it is located nearby a far infrared loop named G172+01, (b) the flux density is found to be three-fold less than that of its ambient interstellar medium surrounding, (c) it is close to the Galactic plane therefore the radiation field is strong and (d) the diameter of the cavity is greater than 1.78^o on IRAS. The dust color temperatures are found to be in the range 21.43 Å 0.18 K to 25.24 Å 4.00 K. Planck's function is found to be non-uniform along its extension and compression, suggesting that the dust and grains are not in the local thermodynamical equilibrium, possibly because of external cause. It is therefore, a deviation from the Gaussian distribution is notated in the histogram of dust color temperature. We conclude that the cavity is formed due to the high pressure events occurred in the past (e.g. AGB wind, supernova explosion)

Supervisor: Prof. Dr. Binil Aryal

MOLECULAR DYNAMICS STUDY OF TRANSPORT PROPERTIES OF CYSTEINE IN WATER

Hem Prasad Bhusal
(July 2018)

ABSTRACT

Molecular dynamics simulation is a prominent way of analyzing the dynamic properties of a system. The molecular dynamics simulation of diffusion, an important transport property, of dilute solution of cysteine in SPC/E water at five different temperatures (288 K, 293 K, 303 K, 313 K, 323 K) under the pressure of 1 bar is studied using GROMACS. OPLS-AA force field parameters are used throughout the simulation. The system under study consists of 3 cysteine molecules (mole fraction 0.003) as solute and 1039 water molecules (mole fraction 0.997) as solvent. The radial distribution functions (RDF's) for five different combinations of atoms of solvent-solvent and solute-solvent molecules are studied for structural analysis. At least two or more distinct peaks are observed in RDF's plots implying that there are interactions between atoms of solvent-solvent and solute-solvent at least up to two co-ordination shells. The co-ordination number of water oxygen around carbonyl oxygen of cysteine is also calculated for five different temperatures. The self-diffusion coefficients of solute and solvent are determined exploiting mean square displacement (MSD) in Einstein's equation. The self-diffusion coefficients are used to calculate the binary diffusion coefficients by means of Darken's relation. The calculated values of self-diffusion and binary diffusion coefficients are compared with available experimental values and they agreed within 12% error. The temperature dependency of diffusions are demonstrated via Arrhenius plots and with the help of these plots activation energies for diffusion are calculated which agreed with experimental results within 13% error.

Supervisor: Prof. Dr. Narayan Pd Adhikari

FIRST-PRINCIPLES STUDY OF ELECTRONIC AND MAGNETIC PROPERTIES OF Ge DOPED HEXAGONAL BORON NITRIDE

Jeewan Panthee
(July 2018)

ABSTRACT

First-Principles calculations to study geometrical structure, stability, electronic properties, and magnetic properties of pristine and Germanium-doped (Ge-doped) hexagonal boron nitride (h-BN) sheets have been carried out. Calculations are based on Density-Functional Theory (DFT) with van der Waals (vdW) interactions in the DFT-D2 approach within Generalized Gradient Approximation (GGA). These calculations are performed using Quantum ESPRESSO (QE) software package. Our study is based on 3 x 3 supercell calculations. The unit cell of h-BN containing one Boron and one nitrogen atom has been used as a basic building block. Among the two possible sites, Boron (B) and Nitrogen(N) sites, of h-BN sheet we find that Germanium impurity is more likely to substitute the boron site (Ge_B) due to low formation energy (7.75 eV). Ge doping severely deforms h-BN sheet, resulting changes the curvature of h-BN sheet around Ge atom. Hence both the doped systems exhibit semi-conducting properties. Present calculations find the band gap of pure h-BN consistent with the previous works. The Ge-doped h-BN, on the other hand, is reduces the band gap to 0.75 eV and 0.45 for Ge_B and Ge_N sites respectively. We also find that the non-magnetic h-BN becomes magnetic via doping of Ge with magnetic moment 1.0 μ_B.

Supervisor: Dr. Nurapati Pantha

AIR POLLUTION DISPERSION MODELING AND ENVIRONMENTAL IMPACT ACCESSMENT OF MITTAL CEMENT INDUSTRY, NEPAL

Jeewan Poudel
(May 2018)

ABSTRACT

The air pollution dispersion pattern of the pollutants emitted from Mittal Cement Industry (MCI) and the local meteorological flow fields around the cement industry have been studied at horizontal grid resolution of 1 km x 1 km covering 70 km x 70 km area centered at MCI. The local meteorological flow fields has been numerically simulated using the state-of-the-art-of-the Weather Research and Forecasting (WRF) model initialized with NCEP 6-hourly meteorological data with a resolution of 1.0° x 1.0°, 24 categories of land use data and 30 second terrain elevation data by United States Geological Survey (USGS). The dispersion pattern of pollutants over the study area has been studied using the comprehensive Chemical Transport Model (CTM). The region near MCI remains calm under strongly stratified boundary layer during the night and early morning hours whereas the afternoon time experience strengthened upslope wind flow towards northern regions through corridors of Kankai, Mechi and Mahananda River. The southeastern region experiences windy situation in the late afternoon where the wind speed reaches up to 23 m/s. The southern places like Patharia, Kechana, Gherabari, Pawa Khali and Dumaria are found relatively warmer than the northern one where the temperature reaches about 31°C in the afternoon. A strong surface inversion lifting up from 200m to 800m till late morning hours confines the pollutants over the study region and the pollutants are weakly dispersed. The turbulence created in the southern plain during the afternoon blows away the pollutants towards Kharra Balbari of Bihar, India. The simulation results of CTM suggest that Haldibari, located near to southwestern region of study area is the most affected place by the pollutants emitted from MCI where concentration of pollutants reaches about 0.5 ppb. The dense forest extending from western to northwestern areas aids in declining pollutant concentration reaching over Shani Arjun and Budhabare areas. The pollutants released from MCI blow through Anarmani, Shani Arjun areas to Budhabare, Shantipur, Suryodaya and finally enters to Mirik of Darjeeling in West Bengal, India in the afternoon.

Supervisor: Prof. Dr. Ram Pd Regmi

CONPARITIVE STUDY ON VIBRATIONAL PROPERTIES OF QUINONE MOLECULES

Kashmir Lamichhane
(Feb 2019)

ABSTRACT

The present work enumerates detailed computational investigation in to vibrational properties of two different quinone family, separately and comparatively in gas phase, which are 1,4 Anhra quinones, and 1,4 Napthoquinone substituted with different side groups infact we compared vibrational properties of six different 1,4– AQ and sever different 1,4–NQ in gas phase. Furthermore we studied 1,4 NQ in both gas and CCl4, where we observed solvent has effect in the carbonyl group but has not constrain the quinone ring structure. In addition to comparative study of different quinones family 1,4–NQ and 1,4–AQ has been done and concluded that addition of an aromatic ring constrain the quinone ring structure but carbonyl group and addition of an aromatic ring added at least a band of in the spectra we had comparative study of different member of same family and concluded that there is slight change of spectra on both frequency shift and intensity of IR activity. In the spectra we observed two band intense (around at 1728 cm^{-1}) and weak (around 1640 cm^{-1}). Calculated IR spectra and corresponding mode of vibration shows that in 1,4 AQ and 1,4–NQ both C = O group were strongly coupled in either gas or CCl_4. Expect MNQ2 there is single intense band and number of weak band, but double intense band observed at MNQ2. Calculation was under taken using the B3LYP functional and the 6–31 G + (d) basis set.

Supervisor: Dr. Hari Prasad Lamichhane

STUDY OF DUST COLOR TEMPERATURE AND DUST MASS OF A FAR INFRARED CAVITY NEARBY KK-LOOP G134+00

Khagendra Katuwal
(December 2018)

ABSTRACT

A systematic search of isolated loop like structure in the far infrared (100μm and 60μm) IRAS (Infrared Astronomical Satellite) survey was performed using Sky View Observatory (http://skyview.gsfc.nasa.gov/). In order to find the possible candidate of isolated structure not yet studied, we used SIMBAD (http://simbad.ustrasbg.fr) database to locate discrete sources in the region. A new isolated far infrared loop like structure nearby KK-loop G265-04 (size 1.7^{o} x 1.5^{o}) at galactic longitude = 265.2^{o} and galactic latitude = -4.20^{o} was found at the distance of about 200 pc. In this present work, we have calculated dust mass, dust color temperature, and studied the distribution of Planck's function. We also studied the flux density variation using software ALADIN V2.5. Our aim was to test whether the dusts in the cavity are in the thermal equilibrium or not. The dust color temperature is found to lie in the range 21.81 ± 0.48 K to 24.48 ± 0.85 K. The Planck's function distribution along the major and minor diameter is found to be fluctuating, suggesting that the cavity might not be in the thermodynamic equilibrium.

Supervisor: Prof. Dr. Binil Aryal

METEOROLOGICAL FLOWS AND AIR POLLUTION DISPERSION MODELING OF UNITED CEMENT FACTORY, DHADING, NEPAL

Krishna Khatri
(August 2018)

ABSTRACT

In this research, we have considered one of the potential sources of the air pollution, namely, the United Cement Factory (UCF), located in the Naubise area about 17 km west to Kathmandu valley as a case study. The winter time meteorology over the Kathmandu valley and its surrounding areas has been numerically simulated using WRF model initialized with the NCEP-FNL and USGS land-use and terrain elevation data. The transport and diffusion of fictitious pollutants released at UCF has been numerically simulated using a comprehensive Chemical Transport Model (CTM) initializing with the meteorological fields prepared from WRF simulation. The WRF simulated meteorological fields suggest that while the Kathmandu valley remains calm or windless from late evening to late morning with strong stratified near surface atmosphere, the Dhading valley also remains stably stratified but significant drainage flow prevails over the area adjacent to the Kathmandu valley. With the development of mixed layer from around 0900 LST two characteristics valley winds intrude into the Kathmandu valley, namely, the northwesterly from the Dhading/Trishuli valley via Thankot-Bhimdhunga-Mudku-Tinpiple low-mountain passes and the southwesterly wind via Bagmati River valley. The two wind converse in the central area of the valley and channel out from the eastern low-mountain passes such as Sangha, Nala, Sankhu. During the late afternoon the northwesterly makes hydraulic jump and overrides the shallow and relatively cooler southwesterly in the central and eastern part of the valley there by develop double layering flow structure. The CTM simulated dynamics of fictitious pollutants suggest that the pollutants released at UCF largely remains stagnant in its vicinities but the southeasterly drainage flow transport the pollutant towards the northeast of Dhading valley. However, from around noontime, the pollutants are effectively transported up into the Kathmandu valley via Nagdhunga/Thankot low-mountain pass until the late evening. If an uncoordinated industrializations and uncontrolled emissions activities continue unabated, emission over the Naubise and associated areas are likely to further deteriorate the air quality of Kathmandu valley.

Supervisor: Prof. Dr. Ram Prasad Regmi

HYDROPHOBICITY OF ETHANE DIMER IN DIFFERENT SOLVENT ENVIRONMENT: A CLASSICAL MOLECULAR DYNAMICS STUDY

Krishna Prasad Gautam
(June 2018)

ABSTRACT

Classical Molecular Dynamics (MD) simulations have been performed for ethane dimer in three different solvents (Water, Methanol, Acetonitrile) using GROMACS (Groningen Machine for Chemical Simulations) software at temperature 298K and 1 bar pressure. Force field parameters are used accroding to CHARMM (Chemistry at HARvard Macromolecular Mechanics). The hydrophobic interactions have been studied in terms of the potential that gives an average force over all configuration of the given system (PMF). The Umbrella Sampling simulation is carried out for 10 ns separately for three different solvents. PMF have been calculated using the weighted histogram analysis method (WHAM). In our results we found two minima where the first minima is called contact minima, second minima is called solvent separated minima and one maxima called desolvation maxima. The first minima (contact minima) is like LJ potential and the second minima (solvent separated minima)is due to the solvent effect in between two ethane dimer. The contact minima, desolation maxima and solvent separated minima are obtained at distance 0.44 nm, 0.60 nm and 0.80 nm for ethane - water system which is consistent with the reference. Similar to the ethane - water system the values are obtained at distance 0.46 nm, 0.66 nm, 0.82 nm and for ethane - methanol system. On the other hand values are obtained at distance 0.46 nm, 0.67 nm, and 0.85 nm for ethane - acetonitrile system. Our study shows the the interaction between ethane dimer is softer in methanol and acetonitrile than in water because of presence of methyl group in methanol and acetonitrile.

Supervisor: Dr. Nurapati Pantha

MESO-SCALE METEOROLOGICAL FLOWS AND AIR POLLUTION DISPERSION MODELING OF Narayani Cement Industry, Parsa, Nepal

Manoj Chhetri
(July 2018)

ABSTRACT

Present study examined the dispersion pattern of pollutants of Narayani Cement Industry (NCI) by releasing fictitious pollutants at its location. The study examines regional scale wintertime meteorological situation over the southern plain area of Central Nepal Himalaya, meteorological implications for air pollution transport and formation of pollutant fields over the area released from the location of NCI. The meteorological flow fields were numerically simulated using the WRF modeling system whereas the CTM simulation provided the dynamics and formation of pollutant fields for fictitious pollutants released at the location of NCI. The meteorological fields were simulated at 1km1km horizontal grid resolution by initializing WRF modeling system with x1 NCEP FNL global meteorological and USGS terrain elevation and land use data sets. Likewise, the CTM model was initialized with the meteorological fields prepared from WRF simulation and the fictitious emission inventory physically equivalent to the PM2:5. The WRF simulated meteorological fields suggest that easterly/northeasterly wind prevails in and around the NCI during the night and morning times over the area in and round the Birgunj. Strong northerly/northeasterly downslope winds from the northern mountainous region swipes the area under highly stratified near surface atmosphere feed by the return flow over the mountains originated from south of NCI. Strong surface inversion (5-6^{o}C) builds up over the area during the early morning that tends to erode only in the late morning, around 1000 LST. The afternoon time mixing height may go up to 2km AGL. The meteorological flow fields show strong diurnal periodicity. The diurnal dispersion patterns of the pollutants released at the NCI resembles with the pattern of meteorological flow fields. The pollutants released at NCI are transported mostly towards the west and southwest during the night and morning times but they are transported towards the northwest/north during the afternoon time. The dynamics of pollutants released NCI suggest that the areas such as Harpataganj, Bairiya Birta, Jaimangalapur, Ramghadawa etc appear to be most affected by the pollutants released by the NCI.

Supervisor: Prof. Dr. Ram Pd Regmi

NEUTRON YIELD AND SCALING LAWS OF THE PLASMA FOCUS DEVICE PFMA1 FOR DIFFERENT PRESSURES

Najin Kadel
(September 2018)

ABSTRACT

A plasma focus device produces hot and dense plasma sufficient for initiating fusion for a very short time. PFMA1 (Plasma Focus for Medical Applications-1) is the first prototype of a new application of the plasma focus technology conceived to produce short-lived radioisotope for medical applications. PFMA1 is a 27 kV, 150 kJ, 95 nH Mather-type plasma focus designed for repetition frequencies up to 1 Hz. It is located at the University of Bologna, Italy. In this work, we have used the Lee Model Code to study neutron yield from the plasma focus device PFMA1, which uses deuterium as a working gas for neutron yield. Numerical experiments are carried out under the various operating pressure of the gas to study the neutron yield with other parameter adjusted to the values considered in experiments conducted in the device. Numerical results obtained using the Lee Model Code is compared with reported experimental data and the discrepancies are analyzed and discussed. The simulated current curve exactly matches the experimental curve for the case of 2 torr. For other values of pressure, neutron yield is calculated; the nature of yield and range of pressure is similar. The peak neutron yield of 1:38 x 10^7 per shot is observed at 1.5 torr for 95 nH inductance and 6.4^{o}F capacitance. Computed current curves versus pressure are presented and discussed particularly in terms the dynamic resistance and the computed gross properties are presented and the variation of these plasma dynamics is discussed to explain the maximization of the neutron yield at the optimum pressure. Our results agree with previous experimental work with slight differences in some of the plasma dynamics.

Supervisor: Prof. Dr. Raju Khanal

STUDY OF PLANCK FUNCTION DISTRIBUTION OF A FAR INFRARED CAVITY USING AKARI SURVEY

Narayan Budhathoki
(Jan 2019)

ABSTRACT

We present a far infrared cavity at AKARI maps nearby GIRL 299+02 cavity discovered on IRAS maps. Since the resolution of AKARI is 16 times higher than IRAS, dynamical distributions of dust can be studied using 90 and 140 m AKARI maps. The position of our cavity is as follows: RA (J2000) = $12^h20^m55^s$, Dec(J2000)= $-60^o39^m02^s$, which is located at 1.7 kpc distance from us. We studied dust color temperature, dust mass and Planck function distributions of the cavity. The dust color temperature is found to lie in the range of 16.9 ± 0.24 K to 17.9 ± 0.26 K. The mass of the dust in the cavity amounts 0.008 M_{sun}. The Planck function distribution is found to be non-uniform along the diameters of the cavity, suggesting that the dusts in the cavity are not in the thermal equilibrium with gas and radiation field.

Supervisor: Prof. Dr. Binil Aryal

TO STUDY DOPING EFFECT ON ELECTRONIC AND MAGNETIC PROPERTIES OF PEROVSKITE TYPE $KTa_{1-x}Mn_xO_3$ (x = 0,0.50,0.67)

Nirmala Adhikari
(August 2018)

ABSTRACT

$KTa_{1-x}Mn_xO_3$ for (x = 0, 0.50, 0.67) is one of the prominent perovskite used as fuel cells, memories devices, photovoltaic devices and spintronic applicatios. In the present work, we have performed the first-principles calculations to study the structural, electronic and magnetic properties of pristine perovskite KTaO3 and Manganese doped $KTa_{1-x}Mn_xO_3$ perovskite system along Ta site of supercell. The calculations are performed in the Density Functional Theory (DFT) under Generalized Gradient Approximation (GGA) implemented by the Quantum ESPRESSO code. Our study based on supercell calculation. Our finding shows that the pure perovskite KTaO3 is indirect band gap semiconductor having band value 2.13 eV which is close agreement with experimental reported value 2.15 eV. In the study of Mn doped system, we observed that there is indirect band gap decrease from 2.13 eV to 0.84 eV at 50 % Mn doped on perovskite $KTa_{0.5}Mn_{0.5}O_3$ along Ta site for 2x1x1 supercell and 0.81 eV at 67 % Mn doped on perovskite $KTa_{0.33}Mn_{0.67}O_3$ along Ta site for 3x1x1 supercell. Further, we have studied the Density of States (DOS) and we found that there is symmetric distribution of DOS for spin-up and spin-down electron states near Fermi level indicating the non-magnetic nature of pure perovskite KTaO3 having net magnetization zero due to the saturation or paring of valence electrons to it's neighboring atoms. Our further investigations show that antisymmetric distribution of DOS for spin-up and spin-down electronic states for Mn doped perovskite $KTa_{1-x}Mn_xO_3$ system. The contribution to total DOS is due to 2p-orbital of Oxygen and 3d-orbital of Manganese atom around the Fermi level. This suggest that, there is existence of magnetic behavior and have magnetic moment 2 μB and 4 μB for 2x1x1 and 3x1x1 supercell respectively which is mainly originated from the contributions of 3d-orbital of implemented Mn impurity. Whole doped system behaves as half metallic, due to spin-up channel that shows semiconducting nature where as spin-down channel shows the metallic nature.

Supervisor: Dr. Gopi Chandra Kaphle

FIRST-PRINCIPLES STUDY OF ELECTRONIC AND MAGNETIC PROPERTIES OF SODIUM(Na) DOPED HEXAGONAL BORON NITRIDE MONOLAYER

Nirmala Shrestha
(September 2018)

ABSTRACT

The density functional theory (DFT) based first-principles calculations have been adopted for the study of geometrical, electronic and magnetic properties of pure and sodium doped hexagonal boron nitride(h-BN) monolayer. Generalized Gradient Approximation (GGA) based exchange correlation functional are used under software package Quantum ESPRESSO (QE), 6.2.0. version. We have replicated the optimized unit cell of h-BN, two atomic system one boron and other nitrogen having lattice parameters ao = bo = 4:74(A) and interlayer spacing of 20A in order to neglect the interlayer interactions, in two dimensions x and y to obtain different supercells. The substrate has two possible sites for sodium doping, one nitrogen site(NaN) and the other boron site (NaB). On doping sodium at the nitrogen site the small sized supercells seem to have metallic behavior while the higher order supercells assume semiconducting nature with largely reduced band gap to 0.36eV, boron site doped sample is also found to be semiconducting in nature for higher order sample with band gap reduced close to 1eV. The formation energies for both site doping have been estimated which predict that boron site doping is more preferable with lower formation energy. Under density of states (DOS) calculations it is evident that the nitrogen site defect is nonmagnetic in nature with symmetric DOS plot, whereas boron site defect is magnetic with unsymmetrical DOS having total magnetization of $2\mu_B$. The magnetism arises due to the redistribution of charge density as a result of adding a sodium atom as an impurity..

Supervisor: Dr. Nurapati Pantha

A STUDY OF FAR INFRARED CAVITY NEARBY KK-LOOP G265-04

Pawan Giri
(July 2018)

ABSTRACT

A systematic search of isolated loop like structure in the far infrared (100mm and 60mm) IRAS (Infrared Astronomical Satellite) survey was performed using Sky View Observatory (http://skyview.gsfc.nasa.gov/). In order to find the possible candidate of isolated structure not yet studied, we used SIMBAD (http://simbad.ustrasbg.fr) database to locate discrete sources in the region. A new isolated far infrared loop like structure nearby KK- loop G265-04 (size 1.7^{o} x 1.5^{o}) at galactic longitude = 265.20^{o} and galactic latitude = -4.2^{o} was found at the distance of about 200 pc. In this present work, we have calculated dust mass, dust color temperature, and studied the distribution of Planck's function. We also studied the flux density variation using software ALADIN V2.5. Our aim was to test whether the dusts in the cavity are in the thermal equilibrium or not. The dust color temperature is found to lie in the range 21.81 ± 0.48 K to 24.48 ± 0.85 K. The Planck's function distribution along the major and minor diameter is found to be fluctuating, suggesting that the cavity might not be in the thermodynamic equilibrium.

Supervisor: Prof. Dr. Binil Aryal

FIRST-PRINCIPLES STUDY OF ELECTRONIC AND MAGNETIC PROPERTIES OF NICKEL DOPED HEXAGONAL BORON NITRIDE MONOLAYER

Prakash Bissokarma
(June 2018)

ABSTRACT

We have carried out the first-principles calculations to study geometrical structure, electronic, magnetic properties, and stability of pristine and Nickel doped hexagonal boron nitride (h-BN) monolayer. The spin polarized calculations are performed within density functional theory (DFT) approximations. The Generalized Gradient Approximation (GGA) based exchange-correlation functional is implemented by Quantum ESPRESSO (QE) version 5.0.1. The unit cell of h-BN contains a boron atom and a nitrogen atom as basic building block of two dimensional (2D) hexagonal structure. Optimized hexagonal lattice parameters of h-BN monolayer is found to be a_0 = b_0 = 2.51 Å and interlayer spacing is taken to be 20 Å to remove the interactions between the layers. We have used replica of this unit cell along x and y directions to get 3 x 3 supercell, which works as a substrate for doping impurity atom (a nickel atom, Ni). There are two possible sites for Ni to replace single atom in h-BN sheet that is boron (B) site and nitrogen (N) site. Hexagonal boron nitride behaves as either half metal or semiconductor depending upon the doping sites. In case of Nickel doped in B site of h-BN (NiB), there is no gap for up spin electronics states but has definite band gap (0.98 eV) for down spin states indicating that the material is half metallic in nature. However, for Ni doped on N site of h-BN (NiN) there exits certain band gap for both the spin orientations, (1.04 eV) for up spin states and (2.60 eV) for down spin states. This band structure resembles with a semiconductor in nature with overall (reduced) band gap, Eg = 0.76 eV. We further calculated the formation energy (EF) of h-BN sheet and found these values as 5.73 eV on B site and 7.73 eV on N site. The results show that there is more likely to create defect at B site rather than at N site of h-BN sheet. The density of states (DOS) calculations finds asymmetric distribution of DOS for spin-up and spin-down electrons near Fermi level which implies that the doped h-BN system is magnetic with total magnetization 1μ_B. It is dissimilar with pure h-BN sheet (which is non-magneic). The magnetism mainly arises due to the redistribution of the charge density in the doped system.

Supervisor: Dr. Nurapati Pantha

A STUDY OF FAR INFRARED CAVITY NEARBY KK LOOP G150+01

Prakash Chalise
(July 2018)

ABSTRACT

A systematic search of cavity like structure in the far infrared (100mm and 60mm) IRAS (Infrared Astronomical Satellite) survey was performed using SkyView Virtual Observatory. We studied physical properties (dust color temperature, Planck's function, dust mass, size, compression and extension, etc.) and their kinematics (dust color temperature and dust mass maps) of a far infrared cavity at RA (J2000) = 14^h 02^m $44{:}3^s$ and DEC (J2000) = $15^0$4' 2". This cavity is found to have the following properties: (a) it is located (<1 degree) nearby a KK-loop named GIRL 150+01, (b) the flux density is found to be three-fold less than that of its ambient Interstellar Medium (ISM) surroundings, (c) it is close to the Galactic plane, and (d) the size of the cavity is greater than 0.5 degree on IRAS map. This cavity is believed to be formed because of high pressure events occurred in the past (e.g., AGB wind, supernova explosion, etc.). The dust color temperatures calculated using IRIS are found to be in the range 22.6 K - 23.8 K. In this cavity, Planck's function is found to be non-uniform along its extension and compression, suggesting the dust and grains are not in the local thermodynamical equilibrium (LTE), possibly because of external cause. Possible explanation of the results has been presented.

Supervisor: Prof. Dr. Binil Aryal

A STUDY OF A FAR-INFRARED CAVITY NEARBY KK-LOOP G117+00

Prakash Chandra Adhikari
(August 2018)

ABSTRACT

We present an analysis of a cavity-like structure of a nearby KK-loop G117+00 in the far-infrared 60 and 100μm IRAS (Infrared Astronomical Satellite) survey carried out using Sky View Virtual Observatory. G117+00 is located at coordinate source R.A.(J2000) = $00^h0.15^m1^s$ and Dec.(J2000)= $63^o12'2''$. We have studied salient physical attributes (dust color temperature, dust mass, Planck's function, comprehension and extension, etc.) and kinematics properties (dust color temperature and dust mass maps) of our region of interest. After a profound study of G117+00, we found the following properties of this cavity: (a) the dust color temperature of the core region is found to lie in the range 21.21K to 22.61K, (b) the size of the cavity is greater than 0.5 degrees on the IRAS, (c) this cavity is located in the nearby KK loop, (d) value of flux densities is found to be less in the core region and more in the peripheral region, and (e) it is close to the galactic plane. The Gaussian plot of the dust mass and dust color temperature reveals that Planck's function is not strictly valid at this cavity; this finding clarifies that dust and grains of G177+00 are not in local thermodynamical equilibrium. In addition, the dust color temperature and dust mass contour map, as expected, evince that the low temperature region has greater density and higher temperature region has lower density. This cavity is believed to be formed due to violent pressure events such as supernova explosions, AGB wind, etc.

Supervisor: Prof. Dr. Binil Aryal

TRANSPORT PROPERTIES OF CARBON DIOXIDE IN WATER, A MOLECULAR DYNAMICS STUDY

Pramod Ghimire
(July 2018)

ABSTRACT

Transport properties of Carbon dioxide and water has been accomplished at five different temperatures within 278-353 K, where Carbon dioxide (0.003 mole fraction) is taken as a solute and water (0.996 mole fraction) (SPC/E model) is taken as a solvent. This study is performed at two different pressures at 200 bar and 1 bar pressure. The solute-solvent, solvent-solvent radial distribution functions (RDF) have been estimated. This RDF's is useful to describe the structural properties. Self diffusion coefficients of both solvent and solute have been determined by mean square displacement (MSD) curve using Einsteins relation. Darkens relation is used to calculate the binary diffusion coefficient. The temperature dependence of diffusion coefficient also have been analyzed. The estimated data for diffusion coefficient agree with experimental data within 20%. Moreover, the temperature dependence of diffusion coefficient has been found to be consistent within Arrhenius behavior. Activation energies are estimated using Arrhenius plots and the estimated values agree within 12.10%.

Supervisor: Prof. Dr. Narayan Pd Adhikari

THE AGE AND KINEMATIC DISTRIBUTIONS OF THE MILKY WAY STELLAR HALO

Raj Kumar Pradhan
(July 2018)

ABSTRACT

We measure largely unknown, the mean azimuthal velocity (vrot), velocity anisotropy (b), and velocity dispersions (σ_r, σ_θ, σ_ϕ) of the Milky Way halo stars within the galactocentric radial distance, $r \leq 15$ kpc. These parameters are crucial for estimating the mass of the Galaxy and understanding its formation history. Although, due to insufficient information about an inaccurate position and tangential motion of the halo stars, the value of anisotropy velocity parameter is difficult to estimate particularly at large galactocentric radius (r). In the last decades, several authors have attempted to measure the velocity anisotropy by using the observed radial velocity of the star alone, they use a Hierarchical Bayesian scheme to marginalize the missing data (the proper motion, and uncertainty- free distance and line-of-sight velocity) to calculate velocity anisotropy. Furthermore, we investigate the metallicity bias in the kinematics of the halo stars. We find that the metal-poor ([Fe/H] < -1.4) and metal-rich ([Fe/H] > -1.4) of Main Sequence Turn-off (MSTO) sample have kinematic bias, i.e. the retrograde and the prograde motion, with the mean difference in their vrot of roughly 40kms In the case of K-Giant stars (KGs) sample, the metallicity bias in kinematics is negligible; so the distinction, in this case, is not clear-cut. Within r < 15 kpc, our sample population MSTOs, and KGs show radially biased. i.e. $\sigma_r > \sigma_\theta$ or σ_ϕ with $\beta < 0.5$. The apparent kinematic dichotomy in the stellar halo supports the co-existence of multiple populations in the galactic halo that could be associated with different formation scenario, i.e. in-situ versus accretion.

Supervisors:
Dr. Prajwal R. Kafle & Dr. Ajay Kumar Jha

EFFECT OF Fe DOPING ON SPIN GAPLESS PROPERTY OF INVERSE HEUSLER ALLOY Mn2CoAl

Ramesh Dhakal
(November 2018)

ABSTRACT

Heusler alloys containing Mn and Co have received growing interest during last decade due to its potential application in the field of spintronics. Employing first principle calculation, we study the effect of Fe doping, at two di erent concentration, on the SGS property of Mn2CoAl by using plane wave pseudo-potential method within PBEsol GGA framework, exploiting density functional theory. The main group element Al is replaced by Fe atoms by following standard site occupation rule for dopant. Electronic structure calculation shows that doping destroy the SGS property of the compound and induce half-metallicity for lower concentration of dopant. The induced half metallic property is destroyed and very small density of states is observed around the Fermi level instead of real gap, when the dopant concentration is increased. It is found that Fe doping increases the magnetization of the system and this value goes on increasing with the increase in the percentage of doping.

Supervisor: Dr. Gopi Chandra Kaphle

MESO-SCALE METEOROLOGICAL FLOWS AND AIR POLLUTION DISPERSION MODELING OF UDAYAPUR CEMENT INDUSTRY, UDAYAPUR NEPAL

Reason Shakya
(August 2018)

ABSTRACT

Using the comprehensive meteorological and chemical transport models, the prevailing meteorological situation and the dispersion pattern of pollutant released by the Udayapur Cement Industries (UCI) were studied. Initializing the Weather Research and Forecasting (WRF) model with the National Center for Environmental Prediction (NCEP) FNL ($1^{o}\times1^{o}$) meteorological and United States Geological Survey (USGS) terrain and land-use data sets, meteorological simulation was carried for 0545 LST 08 March to 0545 LST 11 March 2017 over the triply nested two-way interacting mesh. Utilizing the meteorological fields produced for the finest domain of 1 km ×1 km horizontal grid resolution and the fictitious pollutants released at UCI, Chemical Transport Model (CTM) simulation was performed for 0545 LST 10 March to 0545 LST 11 March, 2017 over the 70 km × 70 km area at 1 km×1 km horizontal resolution. The WRF simulation results suggest that the most prominent wind in and around UCI is the easterly wind and it prevails most of the time except around the midnight. During the period, the northerly down slope wind originating from the northern mountains region penetrates deep into the southern plain. Strong surface inversion develops over the region from the evening that erodes only in the late morning. Daytime mixed layer height may be averaged around 800 m above the ground surface that also collapses frequently with the subside occurring over the area. It is thus concluded that the prevailing meteorology over the area is highly adverse for air pollution. The CTM simulation of fictitious pollutants released at UCI results unveils that the pollutants released by the industry are mostly transported towards the west/southwest except during the early morning time when it is confined with the immediate vicinities of the industry. The pollutants released by the UCI are likely to affect the Golbazar and associated areas and beyond. The northern, eastern and the southeastern part of the study areas are not affected by the pollutants released by the UCI. The CTM simulation can be extensively used to assess the dynamics of pollutants and to develop necessary control system for existing sources and for industrial site prospecting.

Supervisor: Prof. Dr. Ram Pd Regmi

TO STUDY OF STRUCTURAL, ELECTRONIC AND MAGNETIC BEHAVIOR OF Fe DOPED CeCrO3 PEROVSKITE: A FIRST-PRINCIPLES CALCULATION

Reg Bahadur Dangi
(June 2018)

ABSTRACT

We have carried out the first-Principles calculation to study structural, electronic and magnetic properties of pristine and iron doping impurity of the perovskite CeCrO3. The spin-polarization calculations are performed under Density Functional Theory (DFT). From the present calculation, optimized of lattice parameter of CeCrO3 is found to be 3.74Å agrees well experimental value 3.87Å within 3.3% deviation. To calculate the variation of doping iron (Fe) concentration we used 2x1x1 and 3x1x1 supercell propagating along x-direction. In case CeCrO3 unit cell, there is no gap for up spin electronic states but has definite band gap 2.92eV with indirect band for down spin states indicating that the material is half metallic in nature. This estimated of band gap agrees with experimental value of 2.89eV within 1.7% deviations. However supercell behaves as weak half-metallic nature having band gap is 0.14eV with indirect band. After doping, we found that slightly change in electronic and magnetic properties. If the doping concentration 50% and 67% iron impurity at Chromium site of the perovskite CeCr1-xFexO3 system shows that metallic nature. Effect of doping concentration of the impurity reduced the band gap. We have found the unit cell of cubic perovskite CeCrO3 ferromagnetic nature has net magnetic moment 3.88B which agree with experimental value 4 μ_B within 3.3% deviation. Whereas the supercell 2x1x1 found to be weak ferrimagnetic nature while iron doped 50% impurity at chromium of the perovskite CeCr0:50Fe0:50O3 system found ferrimagnetic nature with magnetic moment 1.83 μ_B. Therefore the present investigations show that doping concentration of iron impurity at chromium site reduces the band gap on both supercell. Furthermore there is no gap for up spin and spin down after doped iron impurity atoms indicating the metallic nature. This investigation shows that after doping perovskite system behave metallic nature in all concentration transition. Therefore all pristine and doped perovskite CeCrO3 system has found to have certain magnetic moment it is due to the contributions of 4f and 3d orbitals as these electrons.

Supervisor: Dr. Gopi Chandra Kaphle

MESO-SCALE METEOROLOGICAL FLOWS AND AIR POLLUTION DISPERSION MODELING OF ARGHAKHACHHI CEMENT FACTORY, RUPANDEHI, NEPAL

Rima G.C.
(March 2018)

ABSTRACT

Increased level of air pollution in and around the Lumbini, the UNESCO World Heritage Site is of serious concern. Present study was conceived to understand the wintertime meteorological situations and their implications for air pollution transport over the area, the dynamics of pollutants released by the Arghakhanchi Cement Factory (ACF) located close to the Lumbini and the formation of pollutants over the region. The prevailing wintertime meteorological fields were numerically simulated using the Weather Research and Forecasting (WRF) modeling system initialized with 6 hourly 11 NCEP FNL meteorological and the USGS 1 km x 1 km terrain elevation and 24-catagories land-use data sets. The Eulerian Chemical Transport Model (CTM) was used to simulated the dynamics non-reacting particulate pollutants released by the ACF and the formation of pollutant fields over the 70 km x 70 km area that centers at the location of ACF. The WRF simulation revealed the at land of Lumbini region remains clam or wind less during the night and morning times with strongly stratified immediate atmosphere. Surface inversion begins to build up over the region in the late afternoon (1600 1700 LST) and gradually gets strengthen reaching to as strong as 7C in the early morning that starts to erode only in the late morning (0900 1000 LST). The Butwal-Tansen-Jomsom-Tibetan Plateau appears to be one of the main wind corridors from Gengetic Plain to Tibetan Plateau of the region. The CTM simulation showed that the pollutants released in and around the Lumbini remains stagnated within the surface layer from during the night and morning. The afternoon time westerly/southwesterly wind generally organized the transport of pollutant towards the east and finally towards the north/northeast feeding the pollutants up into the Kaligandaki valley wind that eventually penetrates the Tibetan Plateau. The areas such as Bharirahawa, Butwal, Parashi, Sunawal, Burdhaghat as well as touristic hilltop town Tansen appear to be affected by the pollutants released by the ACF.

Supervisor: Prof. Dr. Ram Pd Regmi

EFFECTS OF ION TEMPERATURE ON MAGNETIZED HELIUM PLASMA SHEATH

Roshan Kumar Thakur
(October 2018)

ABSTRACT

Effects of ion temperature on the magnetized helium plasma sheath have been studied using kinetic trajectory simulation model for the time-independent, collisionless and bounded plasma. The velocity distribution function of the plasma species is considered to be cut-o Maxwellian at the sheath entrance. The ion trajectories are calculated by using the kinetic trajectory simulation method whereas the electrons are considered to obey the Boltzmann distribution. The potential profile, ion density profile, electron density profile and space charge density profile are studied for three different values of normalized ion temperature: 0.1, 0.2 and 0.3. The magnetic field of magnitude 15 mT and obliqueness 300 with normal to the wall are kept constant throughout the simulation. The electrostatic potential decreases towards the wall and has a sharp gradient starting at about 3 electron Debye lengths to the wall and it increases with an increase in ion temperature. The ion and electron density profiles decrease monotonically towards the wall but the decrement of electron density is much faster than that of ions. Furthermore, the decrement of ion and electron density increases with the decrease in ion temperature and hence space charge density is maximum at the wall for the maximum value of ion temperature. The study of ion temperature will give a proper understanding of the sheath properties variation with change in ion temperature. The obtained results are in agreement with previously reported results and useful in various plasma applications such as surface modification, etching, ion implantation, fusion reactors, etc.

Supervisor: Prof. Dr. Raju Khanal

A MOLECULAR DYNAMICS STUDY IN STRUCTURAL DYNAMICS OF A V717I SUBSTITUTION IN THE AMYLOID PRECURSOR PROTEIN

Roshan Shrestha
(November 2018)

ABSTRACT

The effect of Valine to Isoleucine substitution at codon 717 in Amyloid Precursor Protein (APP) is of great importance to understand the stability and properties of mutant beta amyloid peptides in Alzheimer's disease. Alzheimer's disease is a neurodegenerative disorder which leads to the death of nerve cells and hence gradually reduces memory and cognition. One of the prominent features of Alzheimer's disease is the build-up of plaques between nerve cells which are formed when beta amyloid cluster together. These beta amyloids are formed when enzymes act on the APP and are involved in the ability of neurons to change and adapt over time. We have performed Molecular Dynamics (MD) simulations of the wildtype and mutant transmembrane domain of amyloid precursor protein interacting with a model POPC membrane. Here, we present the study in structural dynamics of both mutant and wildtype APP.

Supervisor: Dr. Hari Prasad Lamichhane

ULTRASONOGRAPHIC FINDINGS IN BIOCHEMICALLY HYPOTHYROID PATIENTS

Sandeep Prashad Pant
(June 2018)

ABSTRACT

Ultrasonography (USG) is the most sensitive and satisfactory modality available for examination of thyroid gland and related abnormalities. And chemiluminescence Immunoassay (CLIA) has wide range of applications mainly in environmental monitoring, clinical diagnosis, food safety and pharmaceutical analysis due to exclusive, sensitive, rapid and simple analysis characteristics. A group of 433 samples (F:M = 2.5:1) with USG and thyroid function test (TFT) reports and group of 4438 samples (F:M = 2.6:1) with TFT reports only were studied respectively at Radiology Department and Biochemistry Department of Tribhuvan University Teaching Hospital (TUTH), Kathmandu, Nepal. Subclinical and overt hypothyroidism has had prevalence of 64.58% and 11.73% within 963 hypothyroid samples based on TFTs results only. The mean age and total prevalence for hypothyroidism were respectively 38.9413.60 years and 22.86% with higher prevalence of subclinical hypothyroidism within 140 samples based on USG and TFTs results and that of thyroid dysfunction was 32.56% in females and 5.08% in males within 433 samples based on either USG or TFT reports. Females were more vulnerable towards thyroid dysfunction than that of males. Various magnitude of correlation coefficients including nearly zero, weak, moderate, and strong in both positive and negative directions among FT3, FT4 and TSH concentrations depicted the status of normality in normal samples and severity of abnormality in hypothyroid patients. Various factors involving environmental conditions, demographic locations, genetic effect, status of iodine sufficiency or deficiency were responsible for thyroid disorders.

Supervisor: Dr. Hari Prasad Lamichhane

EFFECT OF ION MACH NUMBER ON ELECTRO-NEGATIVE MAGNETIZED PLASMA SHEATH

Rupesh Kumar Jha
(Jan 2019)

ABSTRACT

The effect of ion Mach number on electro-negative magnetized plasma sheath has been investigated using fluid model. The electro-negative plasma consists of singly charged positive hydrogen ions (H+), negative oxygen ions (O--) electrons and some neutral particles. The electrons and negative ions are in thermal equilibrium and obey Boltzmann distribution. The compiled set of fluid equations are solved for the given boundary conditions. It is found that the ion Mach number has significant effect on the sheath properties. The potential increases at the wall from 68:9 to 87:3 for the ion Mach number changing from 1:0 to 1:5 and it's effect is seen on plasma density profiles. The decreasing rate of negative charged particle density is much faster than the ion density. The velocity of ions increases at the wall from 8:2 to 9:6 on increasing ion Mach number from 1:0 to 1:5. The space charge density and net current density gets shifted towards the sheath edge as the ion Mach number is increased. The obtained results are in agreement with previously reported results. The electro-negative magnetized plasma has useful applications in etching, sputtering, surface modification of materials and many more.

Supervisor: Prof. Dr. Raju Khanal

EFFECT OF OBLIQUENESS ON MAGNETIZED DUSTY PLASMA SHEATH USING KINETIC TRAJECTORY SIMULATION MODEL

Sangeeta Chaulagain
(September 2018)

ABSTRACT

The study of plasma wall transition region is important for all plasma applications since sheath is responsible for the flow of particle and energy towards the wall. It plays an important role in applications like magnetic fusion plasma device, plasma deposition, etching, semiconductor processing, etc. In all cases of plasma dust is present and the study of dust density pro- file, velocity profile, distribution and its impact on potential, electric field, and Lorentz force is necessary to understand in order to design device like ITER, a future tokamak and other fusion devices. A magnetized dusty plasma sheath consisting of ions, electrons and dust is simulated for different obliqueness of magnetic field considering the electrons to follow Boltzmann relation, dust properties by fluid concept and ion properties using the kinetic trajectory simulation model. The density profile, charge density profile, potential profile, electric field profile are studied for different obliqueness of the magnetic field. It has been observed that the increase in obliqueness from 00 to 900 cause the ion density reaching the wall to decrease from 3:56 x 1014 m^{-3} to 2:90 x 1014 m^{-3} whereas electron density is almost constant at the wall. However, no significant change was seen on the dust density profile. Further, a significant change in graph has been seen for the increase in obliqueness in electric field and potential profile at some point near to the wall. On changing the value of obliqueness from 00 to 900 the value of electric field changes from -5766 Vm^{-1} to 5063 Vm^{-1}, The space charge density profile at zero value of obliqueness was compared with Driouch's space charge density profile which has been found to have similar nature.

Supervisor: Prof. Dr. Raju Khanal

EFFECT OF Cr DOPING ON ELECTRONIC AND MAGNETIC PROPERTIES OF INVERSE HEUSLER ALLOY Mn_2CoGa

Sashi Nepal
(June 2018)

ABSTRACT

Heusler compounds have been found to exhibit interesting electronic properties and wide range of magnetic behavior. Many of Heusler compounds have been found to be half-metallic. In this work, we studied the electronic and magnetic properties of inverse Heusler alloy Mn_2CoGa and the effect induced by doping Cr on those properties. We used plane wave pseudo-potential method within DFT framework implemented using Quantum ESPRESSO code. The calculation shows that Mn_2CoGa exhibit weak half metallicity as indicated by availability of tiny amount of states at fermi level below a gap for minority electrons. The calculated total magnetic moment is 2.03 μB/fu which is very close to integral value and thus found to obey established Slater-Pauling rule $M = N_V - 24$ for inverse Heusler compounds. We performed doping at two different concentrations. The empirical rule for atomic occupation established for Heusler alloys says that Cr will occupy D site, but Cr does not follow usual occupation t rule and actually occupies A site. At 25% Cr concentration, calculation shows $Mn_2CoCr0.25Ga0.75$ is a perfect half-metal with typical metallic behavior for majority electrons, but semiconducting behavior with a gap at fermi level for minority electrons. This indicates we can have 100% spin polarization at fermi level. The calculated magnetic moment is 11.0 μB/cell. But calculation at 50% Cr concentration shows that while majority electrons still shows metallic nature, for minority electrons fermi level is slightly shifted into conduction band thus decreasing half-metallicity.

Supervisor: Dr. Gopi Chandra Kaphle

FIRST-PRINCIPLES STUDY OF ELECTRONIC AND MAGNETIC PROPERTIES OF TWO DIMENSIONAL HEXAGONAL BORON NITRIDE DOPED WITH Sn ATOM

Saurabh Lamsal
(Jan 2019)

ABSTRACT

Two dimensional hexagonal Boron Nitride (h-BN) is an inert material in terms of its chemical and electronic properties. When it is doped with impurity atoms significant changes in electronic and magnetic properties have been observed. In this work we studied electronic and magnetic properties of pristine h-BN and Sn doped h-BN sheet by the help of first-principles calculations. We used plane wave pseudo-potential method within DFT framework implemented in Quantum ESPRESSO code using PBE type of functional for exchange correlation energy. We found that pristine h-BN is nonmagnetic wide gap material with a gap of 4.64 eV. The gap was found to be indirect. Substitutional doping of Sn atom at B site (SnB) and at N site (SnN) of a 3×3 h-BN sheet causes severe distortion on geometrical structure of the sheet. In fully relaxed doped system (SnB and SnN), Sn atom lies away from the sheet. For Nitrogen substitution, height of Sn atom from the plane is 2.18°A and that for Boron substitution is 1.97Å. Sn doping at Boron site with low defect formation energy (E_F=9.34 eV) is more feasible than at Nitrogen site (E_F=12.97 eV). Half-metallicity is observed in both systems with vacant states for up spin elctrons and a wide gap of 4.26 eV in SnB. The down spin electrons are metallic in SnN with band gap reduced to 1.85 eV for up spin electrons. Compared to the pristine h-BN, Fermi energy is decreased just by 0.12 eV in SnB whereas it is increased by 1.01 eV in SnN. Magnetic moment of 1μB is observed in both SnB and SnN systems.

Supervisor: Dr. Nurapati Pantha

METEOROLOGICAL FLOWS AND AIR POLLUTION DISPERSION MODELING OF BUTWAL CEMENT INDUSTRY, NAWALPARASI DISTRICT OF NEPAL

Sujan Pokhrel
(August 2018)

ABSTRACT

The dissertation research examined the spatial and temporal characteristics of the meteorological fields and their implication for air pollution transport in 70km × 70km area centered at the Butwal Cement Industry (BCI) as well as the diurnal dynamics of the pollutants released at BCI during the winter season and identified the area's most affected by the BCI. The meteorological flow fields were numerically simulated by using the regional scale Weather Research and Forecasting (WRF) modeling system initialized with the 1° × 1° NCEP meteorological and 25 categories USGS land use and 1km × 1km terrain elevation data. The WRF simulated meteorological field suggests that the plain area of western Nepal in and around the BCI remains rather windy during the night and morning time due to the downslope winds from the northern mountainous areas that intrude deep into the plain under highly stratified immediate atmosphere of the plain area. The area is swiped by the westerly/southwesterly during the later morning to afternoon. The area in and around the BCI remains strongly stratified most of the time except during the afternoon. The afternoon time mixing layer may develop up to the height of 2km AGL. The pollutants released at BCI are largely confined in the close vicinities of the BCI during the early morning. The pollutants are transported towards the southwest reaching to the Lumbini World Heritage Site from late morning to late afternoon. Beyond late afternoon and during the evening the pollutants are transported towards west. From around the midnight the mainstream of the pollutant transport advances towards the southeast affecting the area close to the mountain range. The densely populated urban areas such as Sunawal, Parasi, Ramgram and Bardhaghat as well as the Bhairahawa and Lumbini areas comes under the air pollution airshed of BCI. As the present study remained to be very short-term, it is rather very difficult to generalize both the meteorological flow fields and the air pollution dynamics over the area. A long term investigation usefully complemented by field observations are highly desired..

Supervisor: Prof. Dr. Ram Pd Regmi

ELECTRONIC AND MAGNETIC PROPERTIES OF THE DOUBLE PEROVSKITE $BaLaNiOsO_6$: FIRST-PRINCIPLES STUDY

Sunil Lamichhane
(May 2018)

ABSTRACT

First principles calculations have been performed using Density Functional Theory (DFT) calculation to study the electronic and magnetic properties of newly synthesized double perovskite $BaLaNiOsO_6$. Double perovskite are of great interest because of their novel properties desirable in spintronics applications. We used DFT theory based on WIEN2k code to calculate the electronic and magnetic properties of our system. We used experimentally determined lattice parameter, a = 5.56383 Å, b = c = 5.56383 Å to generate unit cell as well as supercell of system under study. Initially we have used Generalized Gradient Approximation (GGA) with PBE exchange correlation functional for DFT calculations. Although GGA predict Ferromagnetic ground state of materials, GGA unable to provide band gap resemble with experimental work. Then we used Local Density Approximation (LDA) under Density Functional Theory (DFT). Local Density Approximation (LDA) worked surprisingly in our system. After the calculation LDA is found to be more significant than GGA in our system. For Self Consistent Field calculation we used 500 k - points. Band structure calculations and Density of States calculations were done by using modified tetrahedron method. The calculated total energy indicates the ferromagnetic ground state for BaLaNiOsO6 with their easy axis along [0 0 1] direction. We used LDA+U approximation with double corrections as referred by Anisimov et al.. We have chosen localized limit as J = 0 for our investigations. Values of the U, screened coulomb interaction were chosen 5 eV for Ni and 1.25 eV for Os. Then we used Spin orbit Coupling approximation within LDA to account the relativistic correction. LDA predict metallic nature of our system which is against experiment. To overcome this LDA + U approximation was introduced. The sizable strength on spin-orbit coupling in Os plays significant roles in opening the band gap in our system. Our result agrees with the experimental findings (0.35 eV band gap).

Supervisor: Dr. Gopi Chandra Kaphle

STRUCTURAL AND ELECTRONIC PROPERTIES OF PEROVSKITE - TYPE HYDRIDES $MMgH_3$ (M=Na,K)

Tulasi Acharya
(August 2018)

ABSTRACT

Perovskite - type hydrides are of great interest due to their potential application in the field of hydrogen storage systems. We have carried out First-Principles calculations to study structural and electronic properties of perovskite-type hydride $NaMgH_3$ and $KMgH_3$. Further, we have calculated the formation energy of MMgH3 series for different possible reaction pathway. All these calculations were based on Density Functional Theory (DFT) approach within Generalized Gradient Approximation (GGA). We have used Quantum ESPRESSO (QE) software package for the simulation. Optimization of lattice parameters of NaMgH3 found to be *a* = 5.8274 Å, *b* = 7.6872 Å and *c* = 5.7301 (5.4108) Å where a is deviated by 6.77%, b is deviated by 0.205%, and c is deviated by 5.901% with experimental value. Similarly for the $KMgH_3$ we found optimization parameter a = 4.026 (4.023) Å which is deviated by 0.08% by experimental value. Our study convinces that $NaMGH_3$ is an insulator with a direct band gap, E_g, of 2.61 eV at the symmetric point τ whereas $KMgH_3$ is an insulator with indirect bandgap .Eg, of 2.44 eV at the symmetric point X(VBM) and R(CBM). Furthermore DOS plot also follows band structure patterns in the systems. The calculated values of enthalpy also agree with the experimental value for $KMgH_3$. For $NaMgH_3$ it is found to be slightly deviated.

Supervisor: Dr. Gopi Chandra Kaphle

EFFECT OF COLLISION IN MAGNETIZED PLASMA SHEATH

Upama Karki
(July 2018)

ABSTRACT

Plasma sheath has important role in various applications of plasma: thermonuclear fusion, surface modification of materials, fabrication of semiconductor device, sputtering, etching, biomedical and many more. For the case of controlling the plasma in most of the applications now-a-days use magnetic field. In this work, the effect of collision in plasma sheath in the presence of uniform and oblique magnetic field has been investigated using fluid model, where the effect of pressure gradient force term, which is usually neglected, is also taken into account. The plasma consists of hydrogen ions, electrons and neutral hydrogen. The compiled set of dimensionless fluid equations is solved numerically for the given boundary conditions. The results show that collision has considerable effect in ion density and its explicit effect can be seen in velocity and space charge density as well. In addition, it is found that the magnitude of potential increases on the wall with increase in collision frequency and hence the decreasing rate of electron density shifts towards the sheath entrance. Comparison of the results with previous work revealed that the obtained results are in good agreement.

Supervisor: Prof. Dr. Raju Khanal

Masrers' Dissertation at CDP: 1990 to 2018

Central Department of physics compiled a database of masters' dissertation of last 28 years. This was done by listing the hard copies of masters' dissertation that we have at our departmental library. There are 1023 masters' dissertations at the library. A complete list with the title of dissertation, name of students, name of supervisor and the year of viva examination are compiled. Now it is available at the official webpage of CDP (https://tucdp.edu.np/thesis/).

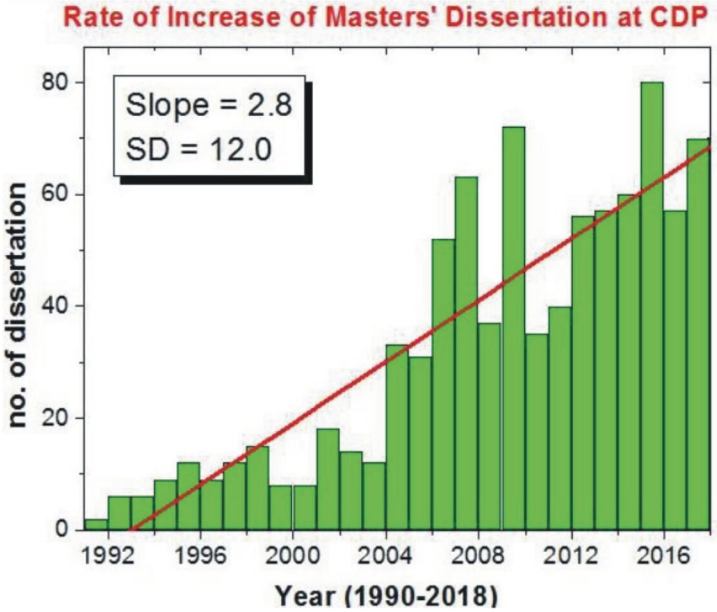


Figure 1: *Rate of increase of masters' dissertation from 1990 to till date. The slope is found to be 5.5. The average number of masters' dissertation is found to be 32 per year.*

Thity nine supervisors and more than 25 co-supervisors have been found to involve in the dissertation supervision of M.Sc. (Physics) students in last 28 yearsOut of this, nine supervisors supervised more than 40 masters' dissertation. These are Prof. Dr. Devendra Raj Mishra, Prof. Dr. Lok Narayan Jha, Prof. Dr. Shekhar Gurung, Prof. Dr. Shesh Kant Aryal, Prof. Dr. Uday Raj Khanal, Prof. Dr. Jeevan Jyoti Nakarmi, Prof. Dr. Binil Aryal, Prof. Dr. Raju Khanal and Prof. Dr. Narayan Pd Adhikari. Electronic files (pdf) of about 50% dissertations are available. The rest 50% dissertations need to be dizitised. CDP is trying to make all dissertations available electronically. CDP have begun scanning dissertations. Mr. Sagar Rawal, a third semester students and his team has done remarkable work in compiling the database. Till date, only the front page, abstract page and evaluation page has been scanned and made it available for all.

. Dissertation is not compulsory in M.Sc. (Physics) till date, mainly because of less number of supervisors in the central department as well as in colleges. The ratio of number of students per faculty at CDP is about 17. In other colleges, this ratio is even larger. Therefore, more research faculty is needed to fulfil this demand.

Table 1: List of supervisors who supervised masters dissertation of CDP students. The last column shows the number of students supervised. The grey shaded shows the supervisor's who supervised more than 40 M.Sc. (Physics) students.

SN	Supervisor's Name	No. of thesis
1	Dr. Ajay Kumar Jha	2
2	Dr. Bal Ram Ghimire	10
3	Dr. Balkrishna Sapkota	11
4	Dr. Bhadra Prasad Pokharel	18
5	Dr. Bidyapati Jha	2
6	Dr. Bimal Prasad Karki	4
7	Dr. Binil Aryal	161
8	Dr. Binod Kumar Bhattarai	10
9	Dr. Buddha Ram Shah	8
10	Dr. Deepak Raj Pant	2
11	Dr. Devendra Raj Mishra	57
12	Dr. Devi Dutta Paudyal	18
13	Dr. Gopi Chandra Kaphle	27
14	Dr. Hari Bahadur Karki	6
15	Dr. Hari Prasad Lamichhane	24
16	Dr. Jeevan Jyoti Nakarmi	88
17	Dr. Kedar Nath Khanal	5
18	Dr. Lok Narayan Jha	52
19	Dr. Mukunda Mani Aryal	28
20	Dr. Nanda Bahadur Maharjan	8
21	Dr. Narayan Pd Adhikari	132
22	Dr. Nurapati Pantha	11
23	Dr. Pradeep Kumar Bhattarai	14
24	Dr. Rajendra Parajuli	4
25	Dr. Raju Khanal	54
26	Dr. Ram Prasad Regmi	38
27	Dr. Sanju Shrestha	15
28	Dr. Shankar Prasad Shrestha	12
29	Dr. Shanta Lall Shrestha	2
30	Dr. Shekhar Gurung	47
31	Dr. Shesh Kanta Aryal	59
32	Dr. Sita Ram Joshi	2
33	Dr. Sitaram Prasad Byahut	14
34	Dr. Surendra Raj Kafle	2
35	Dr. Triratna Bajracharya	2
36	Dr. Uday Raj Khanal	47
37	Dr. Yagya Prasad Dhungana	4
38	Mr. Rajendra Prasad Koirala	12
39	Mr. Tika Ram Lamichhane	7
Total		1023

According to the list at the administration, there should be around 1130 masters' dissertations. About 110 masters' dissertation are not found in the library. The most of them are old one (before 1992). Probably, because of the shift from old building to the new, these dissertations were lost. Now CDP is trying to collect it from individuals and Central Library. A few dissertations are found and added. We hope to compile hard copy as well as soft copy of our M.Sc.(Physics) dissertation within a year.

20 Ph.D. Awarded in Physics

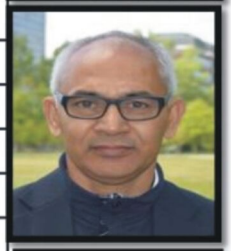
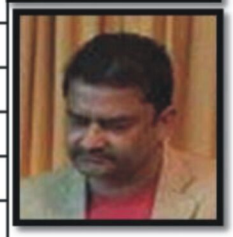







S.N.	Name	Supervisor
1	Dr. Kedar Nath Baral	Prof. Dr. Kedar Lal Shrestha
2	Dr. Jeevan Jyoti Nakarmi	Prof. Dr. Lok Narayan Jha
3	Dr. Nanda Bd Maharjan	Prof. Dr. Devi Dutta Paudel
4	Dr. Sanju Shrestha	Prof. Dr. Pradeep K Bhattarai
5	Dr. Kanchan Pd Adhikari	Prof. Dr. Lok Narayan Jha
6	Dr. Neelam Shrestha	Prof. Dr. Jeevan Jyoti Nakarmi
7	Dr. Indra Bd Karki	Prof. Dr. Jeevan Jyoti Nakarmi
8	Dr. Gopi Chandra Kaphle	Prof. Dr. Narayan Pd Adhikari
9	Dr. Shiv Narayan Yadav	Prof. Dr. Binil Aryal
10	Dr. Nurapati Pantha	Prof. Dr. Narayan Pd Adhikari
11	Dr. Prem Raj Dhungel	Prof. Dr. Udayraj Khanal
12	Dr. Sanat Kumar Sharma	Prof. Dr. Udayraj Khanal
13	Dr. Krishna R Adhikari	Prof. Dr. Shekhar Gurung
14	Dr. Shashit K Yadav	Prof. Dr. Lok Narayan Jha
15	Dr. Ajay Kumar Jha	Prof. Dr. Binil Aryal
16	Dr. Kisori Yadav	Prof. Dr. Jeevan Jyoti Nakarmi
17	Dr. Pitri Bhakta Adhikari	Prof. Dr. Kedar Nath Baral
18	Dr. Ghanshyam Thakur	Prof. Dr. Raju Khanal
19	Dr. Arjun Kumar Gautam	Prof. Dr. Binil Aryal
20	Dr. Saran Lamichhane	Prof. Dr. Narayan Pd Adhikari









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