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CURRICULUM VITAE

EDUCATION:

Indian Institute of Technology Mandi (H.P.), India	Ph.D., Degree in Condensed Matter Physics
H.N.B. Garhwal University Srinagar Uttaranchal, India	M.Sc., Physics
Himachal Pradesh University Shimla, India	B.Sc., Non-Medical

AWARDS AND FELLOWSHIPS:

- Qualified CSIR-UGC JRF NET-2012 and Awarded Junior/Senior Research Fellowship from Govt. of India.
- Qualified Graduate Aptitude Test-2009 (All India Rank-176) & 2012 (All India Rank-29).
- Qualified State Eligibility Test-2011.

RESEARCH INTERESTS:

- To understand the various physical properties such as, structural, electronic, magnetic, transport etc. of strongly correlated materials by using LSDA/GGA (DFT), DFT+U and DFT+DMFT based *ab initio* methods.

TECHNICAL SKILLS:

- Programming skills: Fortran90.
- Application Softwares: Windows, Linux, LATEX, MS-Word, MS-Power point, MS-Excel, XcrysDen, Vesta, Grace etc.
- First principles codes: Elk, WIEN2k, Abinit, Embedded DMFT and Wannier90.

ORIENTATION/REFRESHER/TUTORIALS ATTENDED:

- “*Electronic structure at the cutting edge with the Elk code*”
CECAM, EPFL, Lausanne, Switzerland, August 10th to August 14th, 2015, organized by Sangeeta Sharma, John Kay Dewhurst and E. K. U. Gross, Max Planck Institute of Microstructure Physics, Halle, Germany.
- Completed one week “*TRAINING OF TRAINERS FOR TEACHERS*” from 09 Sep. 2019 to 13 Sep. 2019 at JLN GC HARIPUR MANALI organized by National Institute of Technical Teachers, Training and Research Bhopal.
- Completed one week national workshop on “*Traditional Local Foods in Western Himalaya*” from 16 Nov. 2021 to 22 Nov. 2021 organized by JLN GC Haripur Manali.
- Completed 4 week Orientation programme for “*Faculty in Universities/ Colleges of Higher Education*” from 20 December 2021 to 19 January 2022, from Teaching Learning Centre, Ramanujan College, University of Delhi.
- Completed one-week faculty development programme for “*Faculty in Universities / Colleges of Higher Education*” from 20th December 2023 to 28th December 2023, from SCV Govt College, Palampur, Kangra HP.
- Completed 2 week Orientation programme for “*Faculty in Universities / Colleges of Higher Education*” from 27th February 2023 to 13th March 2023, from Teaching Learning Centre, Ramanujan College, University of Delhi.
- Completed one week Faculty Development Programme on “*Research Methodology and Academic Development*” from 20 June 2024 to 26 June 2024 organized by Himalayan Council for Scientific Research in collaboration with Govt. College Sainj,.

TEACHING EXPERIENCE:

Six years teaching experience of BSc courses in two colleges;

- JLN Govt College Haripur (Manali) 25/06/2018 to 03/12/2021
- Govt College Kullu 04/12/2021 to till now

RESEARCH EXPERIENCE:

IIT Mandi (H.P.), India Ph.D. Research

Thesis Title: Investigation of structural, electronic and magnetic properties of vanadium and chromium spinels by using density functional theory (DFT) and dynamical mean field theory (DMFT)+DFT.

Supervisor: Dr. Sudhir Kumar Pandey

School of Engineering, Indian Institute of Technology Mandi, Kamand-175005, Himachal Pradesh, India

Brief Synopsis of Research:

My Ph.D. synopsis explores structural, electronic and magnetic aspects of strongly correlated vanadium and chromium spinels. Here, we discuss my Ph.D. synopsis briefly into two parts. In part one, we discuss the various issues, while in second part we discuss how to resolve these issues using DFT and DMFT+DFT methods.

Part 1:

In condensed matter physics, it has always been a challenging task to understand the structural, electronic and magnetic properties of a strongly correlated geometrically frustrated systems, where various competing interactions among electron, lattice, orbital and spin degrees of freedom occur. Vanadium spinels, AV_2O_4 and Chromium spinels, ACr_2O_4 ($A \equiv Zn, Cd$ and Mg) are the examples of these systems. In both chromium and vanadium spinels, the structural transition from high temperature cubic phase to low temperature phases are always a contentious issue from last 20 years. Theoretically, different groups have proposed that the Jahn

Teller (JT) effect (for vanadates) and the spin driven JT effect (for chromates) along with various interactions as mentioned above are responsible for this transition. Normally, in some transition metal oxides orbital ordering (OO) have been observed to play an important role for deciding the structural and magnetic properties because both OO and spin ordering are coupled to each other according to Goodenough Kanamori-Anderson rules. However, the OO pattern of the vanadates ($3d^2$ electrons) has been a long issue as different groups have proposed various mechanisms as: i) d_{xz} and d_{yz} OO without spin-orbit coupling (SOC), ii) $d_{xz}+d_{yz}$ and $d_{xz}-d_{yz}$ OO without SOC and iii) the complex uniform ferro-OO of type $d_{xz} \pm id_{yz}$ in presence of SOC at each V sites. In chromates, there is no orbital degree of freedom because of the 3 d^3 electrons in the t_{2g} level. In chromates, magnetic transition and structural transition take place at the same temperature, which is as per expectation because structural transition removes the frustration and open the possibility of magnetic transition. However, in vanadates, structural transition take place at a temperature less than the magnetic transition, which indicates that the certain degrees of geometrical frustration (DGF) is still present in these systems. Frustration index (measure the DGF), defined as $f=|\Theta_{CW}|/T_N$, where $|\Theta_{CW}|$ and T_N are the Curie-Weiss temperature and the magnetic ordering temperature, respectively. The values of f for $ZnV_2O_4 > MgV_2O_4 > CdV_2O_4$ indicates that the ZnV_2O_4 is more and CdV_2O_4 is least frustrated. The experimentally observed values of magnetic moment (MM) per V atom (M_{exp}) for ZnV_2O_4 , MgV_2O_4 and CdV_2O_4 are found to be 0.63, 0.47 and 1.19 μ_B , respectively and are less than the spin MM per V atom ($M_{spin}=2 \mu_B$). If we attribute $\Delta M=M_{spin}-M_{exp}$ as the DGF in these compounds then the order of geometrical frustration become $MgV_2O_4 > ZnV_2O_4 > CdV_2O_4$ and is inconsistent with that arises from f . The small values of M_{exp} are either due to the quantum spin fluctuations or due to the contribution of large negative values of orbital MM per V atom ($M_{orbital}$) in these compounds as proposed by different groups. $M_{orbital}$ for ZnV_2O_4 , MgV_2O_4 and CdV_2O_4 are found to be -0.75, -0.2 and -0.2 μ_B , respectively. By including $M_{orbital}$ also does not improve the inconsistency about the DGF. As we know that the ground state properties of strongly correlated systems have been described by the local spin density approximation (LSDA)/generalized gradient approximation (GGA) plus Hubbard U method, which is now known as DFT+ U method. This method has been found to converge in the local minima and may predict the wrong ground state of the system. Also, in order to know the magnetic ground state of a system, one has to compare the energy of various spin configurations. Normally, it has been found that the MM of magnetic ions for ferromagnetic and anti ferromagnetic (AFM) configurations are different inside the muffin-tin sphere. If no constraint is applied to the moments of the magnetic ions, then a small change in MM may predict the wrong ground state properties of unknown complex systems. In order to understand the various physical properties as mentioned above for these compounds, several groups have proposed different mechanisms. Most of these mechanisms are based on the model calculations, which are fully parameters dependent. The various parameters used in these calculations are not material specific. Similarly, some ab initio electronic structure calculations have also been performed in these systems, where normally U and Hund's coupling (J) are used as a adjustable parameters. There is no systemically comparative studied of these compounds available in the literature, where the parameters, U and J are material specific. Hence, it is important to know the material specific parameters to understand the various comparative study of these spinels. Also, because of naturally static treatment of electronic correlation in DFT+ U approach, it fails to reproduce the spectral properties. For example, it fails to reproduce the experimentally reported quasi-particle peak of $5f$ character of δ -Pu near the Fermi level. Hence, in order to reproduce the spectral and thermodynamic properties of strongly correlated materials, a more sophisticated methods are needed to account the correlation effects beyond these methods. The most successful method is the dynamical-mean-field theory (DMFT), which describe the correlation effects in a periodic lattice by a strongly interacting impurity coupled to a self consistent bath. Merging this with DFT method, DFT+DMFT approach provides more material specific predictions of correlation effects in solids.

Part 2:

In our study, we tried to understand the various issues as mentioned above by using the DFT and DFT+DMFT approach. The ionic sizes are found to play an important role in inducing the cubic to tetragonal distortion in the above mentioned spinels. For vanadium spinels, anti-ferro OO pattern are found with small deviations from d_{xz} and d_{yz} ($d_{xz}+d_{yz}$ and $d_{xz}-d_{yz}$) OO at the neighboring V sites in the global (local octahedral) coordinate system. Also, in these vanadates, the consistency about the DGF, which arises from the f as well as from the MM is achieved by including both orbital and spin angular momenta for calculating the f and MM in vanadium spinels. This work is expected to provide a valuable information in understanding the geometrically frustrated magnetic behaviour for those systems for which the orbital part of the angular momenta are not quenched. We also study the applicability of LSDA+ U method in understanding the electronic and magnetic properties of the ZnV_2O_4 and found that the unconstrained LSDA+ U calculations are not the correct method for predicting the experimentally observed AFM ground state. However, the constrained LSDA+ U calculations, where the MM of every V atoms in ferromagnetic solution is kept same to the self-consistently obtained value of MM in AFM solution give the experimentally reported ground state

for this system. The present study clearly suggests that the constrained LSDA+ U calculations should be preferred, if one wants to predict the real magnetic ground state of an unknown complex system. As an application, we have shown that the constrained DFT+ U method resolves the inconsistency reported by Yaresko [**Phys. Rev. B. 77, 115106 (2008)**] in the theoretically estimated sign of nearest neighbour exchange coupling constant and variation of its magnitude with increasing U in chromates. We also calculate self consistently the material specific parameter U in vanadates, where its utilization is found to explain the degree of localization of electrons. Because of naturally static treatment of electronic correlation in DFT+ U approach, we have used DFT+DMFT method (account the correlation effects beyond DFT+ U) to understand the electronic structure of vanadium spinels. In this approach, we have used the self-consistent calculated material specific parameters, U and J (determined by Yukawa screening λ) from our earlier publication [**Physics Letters A 381: 2117 (2017)**], where the main features, such as insulating band gaps, degree of itinerancy of V $3d$ electrons and position of lower Hubbard band are observed.

In my research work, I have developed expertise about the DFT+ U and DFT+DMFT methods, which have been used to study the various physical properties of d and f electron systems.

PUBLICATIONS:

1. Sihi, A., **Lal, S.**, and Pandey, S. K.. Studying the effect of different exchange correlation functionals on the structural and electronic properties of a half-Heusler NaAuS compound. <https://arxiv.org/abs/1707.08457>. Under review.
2. Dutta, P., **Lal, S.**, and Pandey, S. K.. Studying the occupied and unoccupied electronic structure of LaCoO₃ by using DFT+embedded DMFT method with the calculated value of U . *European Physical Journal B* **91**: 183 (2018).
3. **Lal, S.**, and Pandey, S. K.. Investigation of temperature dependent structural transition in AV₂O₄ (A=Zn, Mg and Cd) compounds by using density functional theory and dynamical mean field theory. Under process.
4. **Lal, S.**, and Pandey, S. K.. Self-consistent evaluation of effective Coulomb interaction U and its utilization to understand the degree of localization of electrons in vanadium spinels. *Physics Letters A* **381**: 2117 (2017).
5. **Lal, S.**, and Pandey, S. K.. Electronic structure study of vanadium spinels by using density functional theory and dynamical mean field theory. *Europhysics Letters* **117**: 37002 (2017).
6. **Lal, S.**, and Pandey, S. K.. Constrained DFT+ U approach for understanding the magnetic behaviour of ACr₂O₄ (A=Zn, Mg, Cd and Hg) compounds. *Physics Letters A* **381**: 917 (2017).
7. **Lal, S.**, and Pandey, S. K.. Role of orbital degrees of freedom in investigating the magnetic properties of geometrically frustrated vanadium spinels. *Computational Materials Science* **126**: 373 (2017).
8. **Lal, S.**, and Pandey, S. K.. The role of ionic sizes in inducing the cubic to tetragonal distortion in AV₂O₄ and ACr₂O₄ (A = Zn, Mg and Cd) compounds. *Materials Research Express* **3**: 116301 (2016).
9. **Lal, S.**, and Pandey, S. K.. Limitations of unconstrained LSDA+ U calculations in predicting the electronic and magnetic ground state of a geometrically frustrated ZnV₂O₄ compound. *Journal of Magnetism and Magnetic Materials* **412**: 23 (2016).
10. **Lal, S.**, and Pandey, S. K.. Density matrix approach to the orbital ordering in the spinel vanadates: A case study. *European Physical Journal B* **87**: 197 (2014).