A. In International Journals

1. Full potential calculation of electronic properties of rutile RO$_2$ (R = Si, Ge, Sn and Pb) compounds via modified Becke Johnson potential

   **Hardev Singh**, Mukhtiyar Singh, Sarvesh Kumar and Manish K. Kashyap


2. Effect of cation substitution on electronic band structure of ZnGeAs$_2$ pnictides: A mBJLDA approach

   **Hardev S. Saini**, Mukhtiyar Singh, Ali H. Reshak and Manish K. Kashyap


3. Emergence of half metallicity in Cr-doped GaP DMS compound within solubility limit

   **Hardev S. Saini**, Mukhtiyar Singh, Ali H. Reshak and Manish K. Kashyap


4. Variation of half-metallicity and magnetism of Cd$_{1-x}$Cr$_x$Z (Z = S, Se and Te) DMS compounds on reducing dilute limit

   **Hardev S. Saini**, Mukhtiyar Singh, Ali H. Reshak and Manish K. Kashyap


5. Accounting Oxygen vacancy for half-metallicity and magnetism in Fe-doped CeO$_2$ Dilute Magnetic Oxide

   **Hardev S. Saini**, Mukhtiyar Singh, Ali H. Reshak and Manish K. Kashyap

6. **Search of half metallicity in VX (X = As, Sb and Bi) compounds for spintronic applications**

   Hardev S. Saini, Mukhtiyar Singh and Manish K. Kashyap


7. **Modified Becke-Johnson approach for governing half metallic ferromagnetism in Cr-doped GaP DMS compound**

   Hardev S. Saini, Mukhtiyar Singh and Manish K. Kashyap


8. **Effect of substituting sp-element on half metallic ferromagnetism in NiCrSi Heusler alloy**

   Mukhtiyar Singh, Hardev S. Saini and Manish K. Kashyap


9. **Effect of atom interchange on half metallicity of AuMnSn Heusler compound**

   Mukhtiyar Singh, Hardev S. Saini and Manish K. Kashyap


10. **Transition from Ferro- to Ferri-magnetic ordering via Mn disorder in NiCoMnGa quaternary Heusler alloy**

    Mukhtiyar Singh, Hardev S. Saini and Manish K. Kashyap

B. In National/International Conference Proceedings

1. Accurate Description of Electronic Band gaps in CdXP₂ (X = Si, Ge and Sn) Ternary Pnictide Semiconductors

**Hardev S. Saini**, Mukhtiyar Singh and Manish K. Kashyap

55th DAE-SSP Symposium, Dec. 26-30, 2010, Manipal University, Manipal (Karnataka), INDIA


2. ab-initio study of electronic band structures of CdBAs₂ (B = Si, Ge and Sn) chalcopyrite compounds

**Hardev S. Saini**, Mukhtiyar Singh and Manish K. Kashyap

International Conference on Advances in Condensed and Nano Materials (ICACNM-2011), Feb. 22-26, 2011, Punjab University, Chandigarh, INDIA.


3. Tuning magnetism in semiconducting Cadmium Chalcogenides via Cr-doping

**Hardev S. Saini**, Mukhtiyar Singh and Manish K. Kashyap

56th DAE-SSP Symposium, Dec. 19-23, 2011, SRM University, Kattankulathur (Tamilnadu), INDIA.


4. High Spin Polarization and Magnetization in NiCrS Heusler alloy

Mukhtiyar Singh, **Hardev S. Saini** and Manish K. Kashyap

55th DAE-SSPS Symposium, Dec. 26-30, 2010, Manipal University, Manipal (Karnataka), INDIA.

5. **First principle prediction of half metallic ferromagnetism in Heusler NiMnZ (Z = P, Ge) compounds**

Mukhtiyar Singh, Hardev S. Saini and Manish K. Kashyap

International Conference on Advances in Condensed and Nano Materials (ICACNM-2011), Feb. 22-26, 2011, Punjab University, Chandigarh, INDIA.


6. **Effect of Atomic Disorder on Half-Metallic Ferromagnetism in Fe$_{3-x}$Cr$_x$Si (x = 0, 0.25, 0.75, 1) Heusler alloys**

Mukhtiyar Singh, Hardev S. Saini and Manish K. Kashyap

56$^{\text{th}}$ DAE-SSPS Symposium, Dec. 19-23, 2011, SRM University, Kattankulathur (Tamilnadu), INDIA


7. **First principle prediction of half metallic ferromagnetism of Cd$_{1-x}$Cr$_x$Te (x = 0.25 and 0.125) Dilute Magnetic Semiconductor**

Hardev S. Saini, Mukhtiyar Singh and Manish K. Kashyap

National Conference on Advances in Physics, Feb. 25-26, 2012, Indian Institute of Technology, Roorkee, Roorkee (Uttarakhand), INDIA