MANJEET KUMAR

Ph.D.

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Manjeet Bhatia | Manjeetkb | mani177105_1 | 0000-0002-6904-3549

STRENGTHS

Computational Chemistry/DFT Software

Quantum Espresso
SIESTA & TranSIESTA
Gaussian
ATK-Virtual Nano lab
MD Simulations
MBN Explorer
DL_Poly

TECHNICAL SKILLS

OS & Scientific software

Window | Linux
OriginLab | LaTeX
HTML CSS | Django

HPC experience

CINECA HPC systems
ISCRA class C project

Programming languages

Shell Scripting
Python | numpy
pandas | scipy
Matplotlib
C/C++ (basic)
Fortran (basic)

Machine Learning

Linear regression
Logistic regression
Gaussian Process
Scikit learn

MOTIVATION

An enthusiastic, adaptive and fast-learning person with a broad and acute interest in condensed matter physics and DFT based calculations. I particularly enjoy working and collaborating with researchers from different disciplines to develop new skills and solve new challenges.

EXPERIENCE

Research Associate | University of Hyderabad, Hyderabad.

Mar 2022 – May 2022 | Hyderabad, India.

- Project: Developing an artificial intelligence-based algorithm for exploring surface reaction mechanisms.

Junior Research Fellow | ABV-IIITM, Gwalior.

Mar 2016 – Oct 2017 | Gwalior, India.

- Project: Ab-initio investigation of structural and electronic properties of Zn (Cd)-VI nanowires.
- Pressure induced phase transitions in nanostructures.
- Electronic, optical and magnetic properties of materials.

Project Fellow | ISSC, University of Pune.

Aug 2014 – Dec 2014 | Pune, India.

- Project: First principles investigations of conductance in photo catalytic materials.
- Optimization of fullerene-porphyrin system.
- Ab-initio Calculations on fullerene-porphyrin system.

EDUCATION

Ph.D. Physics | Department of Physics, University of Milan.

Nov 2017 – Dec 2020 | Milan, Italy.

- Thesis Title: Ab-initio Calculation of the Rates of the Reactions between Volatile Organic Compounds in Wine and Cations for Mass Spectrometry.
- Thesis Supervisor: Prof. Nicola Manini.

M.Phil. Physics | Department of Physics, Pondicherry University.

Aug 2011 – Sep 2013 | Pondicherry, India.

- Thesis Title: Electronic transport through ferroelectric barrier by using density functional theory calculations.
- Thesis Supervisor: Dr. Gangineni Ramesh Babu.

M.Sc. Physics (Hons.) | Department of Physics, Punjab University.

Aug 2006 – Aug 2008 | Chandigarh, India.

SVM | KNN | Decision tree | Random forest | Naive Bayes | K-means | Keras | Neural network

RESEARCH INTERESTS

Condensed Matter Physics

Ab initio Calculations | Electronic Structure Methods

Computational Chemistry | Surface Reactions | Reaction Kinetics | Gas-phase Ion Chemistry | Transport Properties

LANGUAGES

Hindi: Native

English: Professional

Italian: Beginner

REFERENCES

Prof. Nicola Manini
Department of Physics, University of Milan, Via Giovanni Celoria, 16, 20133 Milano MI, ITALY.
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Dr. Franco Biasioli
Department of Food Quality and Nutrition, Research and Innovation Center, Fondazione Edmund Mach, 38010 San Michele all'Adige, TN, Italy.
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Prof. Luca Cappellin
DiSC
Dipartimento di Scienze Chimiche, Universita Degli Studi di Padova, Via Marzolo 1, 35121, Padua, Italy.

- Subjects: Quantum Mechanics, Classical Mechanics, Statistical, Electronics, Mathematical Physics, Electrodynamics, Nuclear Physics, Particle Physics.

PGDCA | CEDTI, New Delhi.

Aug 2004 – Sep 2005 — Dharamshala, India.

- Subjects: Personal Computer System, Business System, System Analysis & Design, Programming in C/C++, Programming in VB, SQL Server, Computer Graphics & Multimedia, and Internet Programming Tools.

B.Sc. | Himachal Pradesh University, India.

Jul 2001 – June 2004 — Dharamshala, India.

- Subjects: Physics, Chemistry, Mathematics.

PUBLICATIONS

Peer-reviewed

1. **Manjeet Bhatia**, Franco Biasioli, Luca Cappellin and Kulvinder Singh, A Quantum-chemical Evaluation of Gas-Phase Proton Affinity, Ionization Energy and Reactivity Parameters for Wine Volatiles, to be submitted in *'Molecules'*.
2. **Manjeet Bhatia**, Nicola Manini, Franco Biasioli, Luca Cappellin, Calculated Rate Coefficients Between CI-MS Reagent Ions and Organosulfur Compounds Causing Food Taints and Off-flavours, *International Journal of Mass Spectrometry*, 478, 116860 2022. (**IF 1.98**)
3. **Manjeet Bhatia**, Nicola Manini, Franco Biasioli, Luca Cappellin, Theoretical Investigation of Charge Transfer from NO^+ and O_2^+ Ions to Wine-Related Volatile Compounds for Mass Spectrometry, *Journal of the American Society for Mass Spectrometry*, 33, 2, 251-264 2022. (**IF 3.11**)
4. **Manjeet Bhatia**, Franco Biasioli, Luca Cappellin, Paolo Piseri, Nicola Manini, Ab-initio calculation of the proton transfer reaction rate coefficients to volatile organic compounds related to cork-taint in wine, *Journal of Mass Spectrometry*, 55(11), e4592, 2020. (**IF 1.98**)
5. **Manjeet Bhatia**, Uma Shankar Sharma, Anurag Srivastava, Chromium Influenced High Magnetic Moment and Half-Metallic Nature of GaN Nanotube, *Journal of Nanoscience and Nanotechnology, Volume 19, Number 7* 2019. (**IF 1.35**)
6. **Manjeet Bhatia**, Md. Shahzad Khan and Anurag Srivastava, Pressure induced phase transition in CdTe nanowire: A DFT study, AIP Conference Proceedings, 1953, 040033 (2018).
7. Md. Shahzad Khan, **Manjeet Bhatia** and Anurag Srivastava, Structural and electronic properties of rectangular CdTe nanowire: A DFT study, AIP Conference Proceedings, 1953, 040136 (2018).
8. **Manjeet Bhatia** and Anurag Srivastava, Band gap and magnetic moment of Ga1-xCrxN, AIP Conference Proceedings, 1832, 090045 (2017).
9. **Manjeet K. Bhatia** and G.Ramesh Babu, Electronic transport across a layered structure of Fe/$\beta-$poly vinylidene fluoride/Fe using DFT calculations, *Journal of Computational Electronics volume 13, pages 613–619* 2014. (**IF 1.81**)

PRESENTATIONS/POSTERS

1. Poster Presentation in TUMIEE Training School, 23 Sep-04 Oct 2019, Rethymno, Crete, Greece.
2. Poster Presentation in Summer School on Advanced Materials and Molecular Modelling, 16 Sep-20 Sep 2019, J. Stefan Institute, Ljubljana, Slovenia.
3. Poster Presentation in 4th International Conference on Nanoscience and Technology (ICONN 2017), SRM University, Kattankulathur-603203, Chennai, India.
4. Poster Presentation in 61st DAE Solid State Physics Symposium (DAE-SSPS December 26-30, 2016), KIIT University, Bhubaneswar, India.

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5. Poster Presentation in 4th International e-workshop on computational condensed matter physics (IWCCMP-2016), November 18-20, 2016, ABV-IIITM, Gwalior, India.
6. Poster presentation, 27th PSSI National Symposium on Plasma Science and Technology, December 2012, Pondicherry University, India.

SCHOOLS/WORKSHOPS

GAUSSIAN Workshop |

20 Jan 2020 – 24 Jan 2020 — Hyderabad, India.

- Introduction to Gaussian: Theory and Practice.

COST-TS-ECOST Training School |

23 Sep 2019 – 04 Oct 2019 — Rethymno, Crete, Greece.

- COST Action 17126 TUMIEE Training School.

QUANTUM ESPRESSO Summer School |

16 Sep 2019 – 20 Sep 2019 — JSI, Ljubljana, Slovenia.

- QUANTUM ESPRESSO Summer School on Advanced Materials and Molecular Modelling.

ICONN 2017 |

09 Aug 2017 – 11 Aug 2017 — SRM University, Chennai.

- 4th International Conference on Nanoscience and Technology.

DAE-SSPS |

26 Dec 2016 – 30 Dec 2016 — KIIT University, Bhubaneswar.

- 61st DAE Solid State Physics Symposium.

IWCCMP |

18 Nov 2016 – 20 Nov 2016 — ABV-IIITM, Gwalior.

- 4th International e-workshop on Computational Condensed Matter Physics.

PSSI National Symposium |

10 Dec 2012 – 13 Dec 2012 — Pondicherry University, Pondicherry.

- 27th PSSI National Symposium on Plasma Science and Technology.

PRIZE & AWARDS

- COST Action CA17126 Trainee Grant €1200, ECOST Association.
- UGC Scholarship for M.Phil. €500, India.
- Higher Secondary Scholarship, €250, India.