Faculty Profile

Name: Dr. Surya Chattopadhyaya

Designation: Professor

Department/Centre: Physics

Phone Number: 09436503751 (M)

Email id: surya_ju@yahoo.com; surya@tripurauniv.ac.in

Educational Qualifications: M.Sc. in Physics, Tripura University, Agartala, Tripura (1994); NET (under CSIR Fellowship Scheme, 1999),
Ph.D. in theoretical Chemical Physics (Molecular Spectroscopy), Jadavpur University, Kolkata, West Bengal (2005)

Areas of Interest: Theoretical Condensed Matter Physics & Materials Science; Electronic structure calculation (DFT), Theoretical Molecular Spectroscopy using Configuration Interaction (CI) approach.

Work Experience

Name of the Organization	Designation	Period		Nature of Post (permanent/ temporary etc.)
		From	To	
Ramkrishna Mahavidyalaya, Kailashahar, Tripura (A Government Degree College Under Govt. of Tripura)	Assistant Professor	22 April 2002	29 January 2009	Permanent
Tripura University	Reader	30 January 2009	29 January 2012	Permanent
Tripura University	Associate Professor	30 January 2012	30 September 2016	Permanent
Tripura University	Professor	01 October 2016	Till date	Permanent

Details about research groups:

(i) Theoretical condensed matter physics & materials science research Lab.

I am currently working as a Professor in the Department of Physics, Tripura University. The current research interest of our group is the quantum mechanical solution of many-electron system under the framework of density functional theory (DFT) to explore different properties, e.g. structural, elastic, thermodynamic, electronic, transport, thermoelectric, magnetic and optical properties of different bulk compounds, diverse nanostructures and 2D materials including their different types of multinary alloys, layered perovakites, spinel compounds and their alloys for finding their areas of microelectronic, optoelectronic, spintronic and mechanical applications.

Laboratory facilities:

Sl No	Name of equipments	Model &Make
1	Workstation	Dell T-440
2	Several Desktop computers and Laptops of High Configuration	Dell and Lenovo

Ph. D. awarded

[1] Dr. Abhijit Nath (Awarded in 2015)

Title of the Thesis: *Quantum Mechanical Studies of the Electronic States and Spectroscopic Properties of Some VIA Intra-group Hetero-nuclear Diatomic Molecules*

[2] Dr. Rahul Bhattacharjee (Awarded in 2019)

Title of the Thesis: *Theoretical Investigation of Structural, Electronic and Optical Properties of Some Binary Compounds and Their Alkaline-Earth Element Doped Ternary Alloys Employing Density Functional Theory (DFT) Based FP-LAPW Methodology*

Research scholars registered

[1] Mr. Manish Debbarma (Registered in 2018)

Title of the Thesis: *Density functional theory (DFT) based investigations of physical properties of some mercury (Hg) doped alkaline-earth and transition metal chalcogenide ternary alloys.*

[2] Mr. Utpal Sarkar (Registered in 2018)

Title of the Thesis: *Calculations of physical properties of some alkaline-earth element doped transition metal chalcogenide ternary alloys using density functional theory (DFT) based full-potential linearized augmented plane wave (FP-LAPW) methodology.*

[3] Ms. Debankita Ghosh (Registered in 2018)

Title of the Thesis: *First principle based theoretical investigation of physical properties of some chalcogenide ternary and quaternary alloys containing alkaline-earth and transition metal elements.*

[4] Ms. Sayantika Chanda (Registered in 2018)

Title of the Thesis: *Theoretical investigation of physical properties of some chalcogenide ternary and quaternary alloys containing elements of transition metal group using density functional theory (DFT) based full-potential linearized augmented plane wave (FP-LAPW) approach*

[5] Mr. Bimal Debnath (Registered in 2020)

Title of the Thesis: *Density functional investigations on physical properties of some binary alkaline-earth chalcogenide compounds and their different types of ternary alloys*

[6] Mr. Subhendu Das (Registered in 2021)

Title of the Thesis: *Density functional calculations of physical properties of different type of perovskite compounds and their alloys*

List of Publications

1. Positron impact ionisation of He+ ion
Biswajit Nath, **Surya. Chattopadhyaya**, Chandana Sinha
Eur. Phys. J. D 11, 31-36 (2000)
https://doi.org/10.1007/s100530070102

2. Ab initio Based Configuration Interaction Study of the Electronic Spectrum of GeS
Antara Dutta, **Surya Chattopadhyaya**, Kalyan Kumar Das
J. Phys. Chem. A 105 (2001) 3232-3239
https://doi.org/10.1021/jp002650v

3. Electronic Spectrum of Silicon Monosulfide: Configuration Interaction Study
Surya Chattopadhyaya, Anjan Chattopadhyay, Kalyan Kumar Das
J. Phys. Chem. A 106 *(*2002) 833-841
https://doi.org/10.1021/jp013332e

4. Configuration Interaction Study of the Low-Lying Electronic States of GaBi
Anjan Chattopadhyay, **Surya Chattopadhyaya** and Kalyan Kumar Das
J. Phys. Chem. A 106 (2002) 2685-2694
https://doi.org/10.1021/jp013582v

5. Electronic spectrum of SiO^+: a theoretical study
Surya Chattopadhyaya, Anjan Chattopadhyay, Kalyan Kumar Das
Journal of Molecular Structure (Theochem) 639 (2003) 177–185
https://doi.org/10.1016/j.theochem.2003.08.007

6. Configuration Interaction Study of the Low-Lying Electronic States of Silicon Monoxide
Surya Chattopadhyaya, Anjan Chattopadhyay, and Kalyan Kumar Das
J. Phys. Chem. A 107 (2003) 148-158
https://doi.org/10.1021/jp021845v

7. Low-lying electronic states of InBi: a configuration interaction study
Anjan Chattopadhyay, **Surya Chattopadhyaya**, Kalyan Kumar Das
Journal of Molecular Structure (Theochem) 625 (2003) 95–109
https://doi.org/10.1016/S0166-1280(03)00007-1

8. Electronic states of SiSe: a configuration interaction study
Surya Chattopadhyaya, Kalyan Kumar Das
Chemical Physics Letters 382 (2003) 249–257
https://doi.org/10.1016/j.cplett.2003.10.094

9. Multireference configuration interaction study of the low-lying electronic states of SiS^+
Surya Chattopadhyaya and Kalyan Kumar Das
J. Phys. B: At. Mol. Opt. Phys. 37 (2004) 3355–3367
https://doi.org/10.1088/0953-4075/37/16/011

10. Electronic spectrum of $SiSe^{+}$: a MRDCI study
Surya Chattopadhyaya, Kalyan Kumar Das
Chemical Physics Letters 399 (2004) 140–146
https://doi.org/10.1016/j.cplett.2004.09.110

11. Electronic States and Spectroscopic Properties of SiTe and $SiTe^{+}$
Surya Chattopadhyaya, Anup Pramanik, Amartya Banerjee, and Kalyan Kumar Das
J. Phys. Chem. A 110 (2006) 12303-12311
https://doi.org/10.1021/jp062610c

12. Configuration interaction study of the electronic states and spectroscopic properties of selenium monoxide
Surya Chattopadhyaya*, Abhijit Nath, Kalyan Kumar Das
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 89 (2012) 160- 167
https://doi.org/10.1016/j.saa.2011.12.044

13. Theoretical studies of the electronic spectrum of tellurium monosulfide
Surya Chattopadhyaya*, Abhijit Nath, Kalyan Kumar Das
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 112 (2013) 283–289
https://doi.org/10.1016/j.saa.2013.04.060

14. Electronic states of selenium monosulfide- a theoretical study
Abhijit Nath and **Surya Chattopadhyaya***
Recent Trends in Physics Research (2012)

15. Theoretical investigation of electronic states and spectroscopic properties of tellurium selenide molecule employing relativistic effective core potentials
Surya Chattopadhyaya*, Abhijit Nath, Kalyan Kumar Das
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 124 (2014) 618–628
https://doi.org/10.1016/j.saa.2014.01.032

16. Effects of spin–orbit coupling on the electronic states and spectroscopic properties of tellurium monoxide molecule – A theoretical study
Surya Chattopadhyaya*, Abhijit Nath, Kalyan Kumar Das
Computational and Theoretical Chemistry 1084 (2016) 75–87
https://doi.org/10.1016/j.comptc.2016.03.026

17. Effects of spin–orbit coupling on the electronic states and spectroscopic properties of diatomic SeS
Surya Chattopadhyaya*, Abhijit Nath and Kalyan Kumar Das
J. Phys. B: At. Mol. Opt. Phys. 49 (2016) 065101
https://doi.org/10.1088/0953-4075/49/6/065101

18. Electronic states and spectroscopic properties of MgH in absence and presence of spin–orbit coupling − a configuration interaction study
Surya Chattopadhyaya*
Molecular Physics 20 (2016) 3026-3039
https://doi.org/10.1080/00268976.2016.1213911

19. FP-LAPW methodology based theoretical investigation of structural, electronic and optical properties of $Ba_xPb_{1-x}S$, $Ba_xPb_{1-x}Se$ and $Ba_xPb_{1-x}Te$ ternary alloys
SuryaChattopadhyaya*, Rahul Bhattacharjee
Journal of Physics and Chemistry of Solids 100 (2017) 57–70
http://dx.doi.org/10.1016/j.jpcs.2016.09.005

20. Theoretical study of structural, electronic and optical properties of $Ba_xPb_{1-x}S$, $Ba_xPb_{1-x}Se$ and $Ba_xPb_{1-x}Te$ ternary alloys using FP-LAPW approach
Surya Chattopadhyaya*, Rahul Bhattacharjee
Journal of Alloys and Compounds 694 (2017) 1348e1364
http://dx.doi.org/10.1016/j.jallcom.2016.10.096

21. DFT based FP-LAPW investigation of structural, electronic and optical properties of $Sr_xPb_{1-x}S$, $Sr_xPb_{1-x}Se$ and $Sr_xPb_{1-x}Te$ ternary alloys
Surya Chattopadhyaya*, Rahul Bhattacharjee
Journal of Alloys and Compounds 698 (2017) 868-882
http://dx.doi.org/10.1016/j.jallcom.2016.12.182

22. Theoretical investigation of structural, electronic and optical properties of $Mg_xBa_{1-x}S$, $Mg_xBa_{1-x}Se$ and $Mg_xBa_{1-x}Te$ ternary alloys using DFT based FP-LAPW approach
Rahul Bhattacharjee, **Surya Chattopadhyaya***
Journal of Physics and Chemistry of Solids 110 (2017) 15–29
http://dx.doi.org/10.1016/j.jpcs.2017.05.015

23. Effects of barium (Ba) doping on structural, electronic and optical properties of binary strontium chalcogenide semiconductor compounds - A theoretical investigation using DFT based FP-LAPW approach
Rahul Bhattacharjee, **Surya Chattopadhyaya***
Materials Chemistry and Physics 199 (2017) 295-312
http://dx.doi.org/10.1016/j.matchemphys.2017.06.057

24. Effects of doping of calcium atom(s) on structural, electronic and optical properties of binary strontium chalcogenides - A theoretical investigation using DFT based FP-LAPW methodology
Rahul Bhattacharjee, **Surya Chattopadhyaya***
Solid State Sciences 71 (2017) 92-110
http://dx.doi.org/10.1016/j.solidstatesciences.2017.06.010

25. Tuning of electronic band gaps and optoelectronic properties of binary strontium chalcogenides by means of doping of magnesium atom(s)- a first principles based theoretical initiative with mBJ, B3LYP and WC-GGA functionals
Bimal Debnath, Utpal Sarkar, Manish Debbarma, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Physica B: Physics of Condensed Matter 530 (2018) 53–68
https://doi.org/10.1016/j.physb.2017.10.014

26. Modification of band gaps and optoelectronic properties of binary calcium chalcogenides by means of doping of magnesium atom(s) in rock-salt phase- a first principle based theoretical initiative
Bimal Debnath, Utpal Sarkar, Manish Debbarma, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Journal of Solid State Chemistry 258 (2018) 358–375
https://doi.org/10.1016/j.jssc.2017.10.028

27. Effects of doping of mercury atom(s) on optoelectronic properties of binary zinc chalcogenides - A first principle based theoretical investigation
Manish Debbarma, Utpal Sarkar, Bimal Debnath, Debankita Ghosh, Sayantika Chanda, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Journal of Alloys and Compounds 748 (2018) 446-463
https://doi.org/10.1016/j.jallcom.2018.03.093

28. Influence of doping of mercury atom(s) on optoelectronic properties of binary cadmium chalcogenides - A density functional theory based investigation with different exchange-correlation functionals and including spin-orbit coupling
Manish Debbarma, Utpal Sarkar, Bimal Debnath, Sayantika Chanda, Debankita Ghosh, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Current Applied Physics 18 (2018) 698–716
https://doi.org/10.1016/j.cap.2018.03.010

29. Optoelectronic properties of $Ca_xBa_{1-x}X$ (X=S, Se and Te) alloys: A first principles investigation employing modified Becke-Johnson (mBJ) functional
Bimal Debnath, Manish Debbarma, Debankita Ghosh, Sayantika Chanda, Rahul Bhattacharjee and **Surya Chattopadhyaya***
International Journal of Modern Physics B 33 (2019) 1950042
DOI: https://doi.org/10.1142/S0217979219500425

30. First principle based calculations of the optoelectronic features of HgS_xSe_{1-x}, HgS_xTe_{1-x} and $HgSe_xTe_{1-x}$ alloys with GGA+U functional
Manish Debbarma, Bimal Debnath, Debankita Ghosh, Sayantika Chanda,
Rahul Bhattacharjee, **Surya Chattopadhyaya***
Journal of Physics and Chemistry of Solids 131 (2019) 86–103
https://doi.org/10.1016/j.jpcs.2019.03.009

31. Density functional calculations of structural, elastic and optoelectronic features of $Mg_xZn_{1-x}S$, $Mg_xZn_{1-x}Se$ and $Mg_xZn_{1-x}Te$ alloys
Utpal Sarkar, Bimal Debnath, Manish Debbarma, Debankita Ghosh, Sayantika Chanda, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Materials Chemistry and Physics 230 (2019) 54–77
https://doi.org/10.1016/j.matchemphys.2019.03.050

32. Density functional study of structural, elastic, electronic and optical properties of $Be_xCd_{1-x}S$, $Be_xCd_{1-x}Se$ and $Be_xCd_{1-x}Te$ alloys using FPLAPW approach
Surya Chattopadhyaya*, Utpal Sarkar, Bimal Debnath, Manish Debbarma,
Debankita Ghosh, Sayantika Chanda, Rahul Bhattacharjee
Physica B: Condensed Matter 563 (2019) 1–22
https://doi.org/10.1016/j.physb.2019.03.025

33. Structural, elastic and optoelectronic characteristics of $Be_xZn_{1-x}S$, $Be_xZn_{1-x}Se$ and $Be_xZn_{1-x}Te$ alloys-a density functional based FP-LAPW study

Surya Chattopadhyaya*, Utpal Sarkar, Bimal Debnath, Manish Debbarma, Debankita Ghosh, Sayantika Chanda, Rahul Bhattacharjee

Computational Condensed Matter (ELSEVIER) 20 (2019) e00384

https://doi.org/10.1016/j.cocom.2019.e00384.

34. First principles investigations of structural and optoelectronic properties of cubic $Mg_xZn_{1-x}Se_yTe_{1-y}$ quaternary semiconductor alloys using FP-LAPW approach

Debankita Ghosh, Sayantika Chanda, Bimal Debnath, Manish Debbarma, Rahul Bhattacharjee, **Surya Chattopadhyaya***

Applied Physics A (SPRINGER) 125 (2019) 644

https://doi.org/10.1007/s00339-019-2938-5

35. Structural and optoelectronic properties of cubic $Mg_xZn_{1-x}S_yTe_{1-y}$ semiconductor quaternary alloys-a first principles investigation

Debankita Ghosh, Sayantika Chanda, Bimal Debnath, Manish Debbarma, Rahul Bhattacharjee, **Surya Chattopadhyaya***

Physica B (ELSEVIER) 574 (2019) 411669

https://doi.org/10.1016/j.physb.2019.411669

36. Calculations of the structural and optoelectronic properties of cubic $Cd_xZn_{1-x}Se_yTe_{1-y}$ semiconductor quaternary alloys using the DFT-based FP-LAPW approach

Sayantika Chanda, Debankita Ghosh, Bimal Debnath, Manish Debbarma, Rahul Bhattacharjee, **Surya Chattopadhyaya***

Journal of Computational Electronics (SPRINGER) (2019)

https://doi.org/10.1007/s10825-019-01409-0

37. Density Functional Investigations of Structural, Mechanical and Optoelectronic Properties of BeS_xSe_{1-x}, BeS_xTe_{1-x} and $BeSe_xTe_{1-x}$ Ternary Alloys

Bimal Debnath, Manish Debbarma, Debankita Ghosh, Sayantika Chanda, Rahul Bhattacharjee, **Surya Chattopadhyaya***

Journal of Electronic Materials (SPRINGER) 49 (2020) 1372

https://doi.org/10.1007/s11664-019-07820-4

38. First principle investigations of structural and optoelectronic features of cubic $Cd_xZn_{1-x}S_yTe_{1-y}$ quaternary semiconductor alloys

Sayantika Chanda, Debankita Ghosh, Bimal Debnath, Manish Debbarma,
Rahul Bhattacharjee, **Surya Chattopadhyaya***
Optik - International Journal for Light and Electron Optics (ELSEVIER) 201 (2020) 163510
https://doi.org/10.1016/j.ijleo.2019.163510

39. Structural, mechanical and optoelectronic features of cubic $Mg_xCd_{1-x}S$, $Mg_xCd_{1-x}Se$ and $Mg_xCd_{1-x}Te$ semiconductor ternary alloys: Theoretical investigations using density functional FP-LAPW approach

Utpal Sarkar, Bimal Debnath, Manish Debbarma, Debankita Ghosh,
Sayantika Chanda, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Computational Condensed Matter (ELSEVIER) 22 (2020) e00448
https://doi.org/10.1016/j.cocom.2019.e00448

40. Structural, mechanical and optoelectronic properties of cubic $Be_xMg_{1-x}S$, $Be_xMg_{1-x}Se$ and $Be_xMg_{1-x}Te$ semiconductor ternary alloys: a density functional study

Bimal Debnath, Manish Debbarma, Debankita Ghosh, Sayantika Chanda, Rahul Bhattacharjee,
Surya Chattopadhyaya*
Bulletin of Materials Science (SPRINGER) 43 (2020) 59
https://doi.org/10.1007/s12034-019-2006-y

41. Density Functional Calculations of Elastic and Thermal Properties of Zinc-Blende Mercury–Cadmium-Chalcogenide Ternary Alloys

Manish Debbarma, Subhendu Das, Bimal Debnath, Debankita Ghosh, Sayantika Chanda,
Rahul Bhattacharjee, **Surya Chattopadhyaya***
Metals and Materials International (SPRINGER) (2020)
https://doi.org/10.1007/s12540-020-00778-7

42. First principle investigations of structural, electronic and magnetic properties of Cr doped zinc-blende MgTe ternary alloys with DFT based
FP-LAPW approach

Subhendu Das, **Surya Chattopadhyaya***, Rahul Bhattacharjee

Materials Today: Proceedings 46 (2021) 6324.
https://doi.org/10.1016/j.matpr.2020.05.491

43. A theoretical investigation of structural, electronic and optical properties of wurtzite $Be_xZn_{1-x}O$ ternary alloys using DFT based FP-LAPW approach
Debankita Ghosh, **Surya Chattopadhyaya***
Materials Today: Proceedings 46 (2021) 6295.
https://doi.org/10.1016/j.matpr.2020.05.212

44. First principle investigation of structural, electronic and optical properties of $Mg_xZn_{1-x}S$ hexagonal wurtzite ternary alloys
Utpal Sarkar, **Surya Chattopadhyaya***
Materials Today: Proceedings (ELSEVIER) 46 (2021) 6207.
https://doi.org/10.1016/j.matpr.2020.04.523

45. Density functional calculations of elastic and thermal properties of zinc-blende HgS_xSe_{1-x}, HgS_xTe_{1-x} and $HgSe_xTe_{1-x}$ ternary alloys
Computational Condensed Matter (ELSEVIER) 24 (2020) e00482
Manish Debbarma, Subhendu Das, Bimal Debnath, Debankita Ghosh, Sayantika Chanda, Rahul Bhattacharjee, **Surya Chattopadhyaya***
https://doi.org/10.1016/j.cocom.2020.e00482

46. Theoretical study of optoelectronic properties of hexagonal wurtzite $Cd_xZn_{1-x}O$ ternary alloys using modified Becke-Johnson (mBJ)-GGA Functional
Sayantika Chanda, **Surya Chattopadhyaya***
Materials Today: Proceedings (ELSEVIER) 46 (2021) 6392
https://doi.org/10.1016/j.matpr.2020.06.136

47. Cationic and anionic concentration dependent elastic properties of zinc blende specimens within $Cd_xZn_{1-x}S_ySe_{1-y}$ quaternary system: Calculations with density functional theory
Sayantika Chanda, Manish Debbarma, Debankita Ghosh, Subhendu Das, Bimal Debnath, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Solid State Communications (ELSEVIER) 322 (2020) 114050
https://doi.org/10.1016/j.ssc.2020.114050

48. Density functional study on structural and optoelectronic properties of cubic $Mg_xZn_{1-x}S_ySe_{1-y}$ semiconductor quaternary alloys
Debankita Ghosh, Sayantika Chanda, Bimal Debnath, Manish Debbarma, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Pramana-Journal of Physics (SPRINGER), 94 (2020) 120.
https://doi.org/10.1007/s12043-020-01975-0

49. Density functional study of elastic and thermal properties of cubic mercury-zinc-chalcogenide ternary alloys
Manish Debbarma, Subhendu Das, Bimal Debnath, Debankita Ghosh, Sayantika Chanda, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Bulletin of Materials Science (SPRINGER), 43 (2020) 268.
https://doi.org/10.1007/s12034-020-02236-x

50. First-principle calculations of structural and optoelectronic properties of cubic $Cd_xZn_{1-x}S_ySe_{1-y}$ quaternary alloys with modified Becke-Johnson (mBJ) functional
Sayantika Chanda, Debankita Ghosh, Bimal Debnath, Manish Debbarma, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Indian Journal of Physics (SPRINGER) (2020).
https://doi.org/10.1007/s12648-020-01880-7

51. Beryllium (Be) composition dependent structural and optoelectronic characteristics of wurtzite $Be_xMg_{1-x}S$ ternary alloys: First principle calculations with FP-LAPW scheme
Bimal Debnath, Debankita Ghosh, Manish Debbarma, Sayantika Chanda, Subhendu Das, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Materials Chemistry and Physics (ELEVIER) 258 (2021) 123946.
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52. Cationic and anionic composition-dependent mechanical and thermal properties of zinc-blende specimens under $Mg_xZn_{1-x}S_ySe_{1-y}$ quaternary system: calculations with density functional FP-LAPW scheme
Debankita Ghosh, Manish Debbarma, Sayantika Chanda, Bimal Debnath, Rahul Bhattacharjee, Subhendu Das, **Surya Chattopadhyaya***
The European Physical Journal B (SPRINGER) (2021).

https://doi.org/10.1140/epjb/s10051-020-00024-4

53. First-principles investigations of composition-dependent mechanical properties of zinc-blende constituents of $Mg_xZn_{1-x}S_yTe_{1-y}$ rectangular quaternary system
Debankita Ghosh, Sayantika Chanda, Manish Debbarma, Bimal Debnath, **Surya Chattopadhyaya***
Indian Journal of Physics (SPRINGER) (2021).
https://doi.org/10.1007/s12648-021-02013-4

54. Calculations of selenium and cadmium concentration dependent elastic and thermal properties of zinc-blende specimens under $Cd_xZn_{1-x}Se_yTe_{1-y}$ quaternary system with density functional theory
Sayantika Chanda, Manish Debbarma, Debankita Ghosh, Subhendu Das, Bimal Debnath,
Rahul Bhattacharjee, **Surya Chattopadhyaya***
Materials Today Communications (ELSEVIER) 27 (2021) 102136.
https://doi.org/10.1016/j.mtcomm.2021.102136

55. Structural and optoelectronic properties of cubic $Zn_{1-x-y}Be_xMg_ySe$ quaternary alloys nearly lattice matched to GaAs substrate: A density functional investigation.
Debankita Ghosh, Manish Debbarma, Sayantika Chanda, Bimal Debnath, Subhendu Das,
Rahul Bhattacharjee, **Surya Chattopadhyaya***
Materials Science in Semiconductor Processing (ELSEVIER), 130 (2021) 105803.
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56. Theoretical investigation of magnesium and selenium concentration dependent elastic properties of zinc blende specimens under the $Mg_xZn_{1-x}Se_yTe_{1-y}$ quaternary system with density functional FP-LAPW approach.
Debankita Ghosh, Sayantika Chanda, Manish Debbarma, Bimal Debnath, **Surya Chattopadhyaya***
Mechanics of Materials (ELSEVIER), 158 (2021) 103840.
https://doi.org/10.1016/j.mechmat.2021.103840

57. Composition dependence in mechanical properties of zinc-blende compounds associated with the $Cd_xZn_{1-x}S_yTe_{1-y}$ system: a density functional study.
Sayantika Chanda, Manish Debbarma, Debankita Ghosh, Bimal Debnath, **Surya Chattopadhyaya***
Bulletin of Materials Science (SPRINGER), 2021.
https://doi.org/10.1007/s12034-021-02372-y

58. First principle calculations of structural, elastic, electronic and optical properties of cubic $Cd_{1-x-y}Zn_xHg_yTe$ triangular quaternary alloys and their compounds
Sayantika Chanda, Manish Debbarma, Debankita Ghosh, Bimal Debnath, **Surya Chattopadhyaya***
Physica B: Physics of Condensed Matter (ELSEVIER), 614 (2021) 412999.
https://doi.org/10.1016/j.physb.2021.412999

59. First-Principles Investigation of Structural, Elastic, Electronic and Optical Properties of $Cd_{1-x-y}Zn_xHg_yS$ Quaternary Alloys.
Sayantika Chanda, Manish Debbarma, Debankita Ghosh, Bimal Debnath, **Surya Chattopadhyaya***
Journal of Electronic Materials (SPRINGER) (2021)
https://doi.org/10.1007/s11664-021-08986-6

60**.** Investigation of structural, mechanical and optoelectronic properties of cubic $Cd_{1-x-y}Zn_xHg_ySe$ quaternary alloys through first-principle calculations.
Sayantika Chanda, Manish Debbarma, Debankita Ghosh, Bimal Debnath, **Surya Chattopadhyaya***
Bulletin of Materials Science (SPRINGER) (2022).
https://doi.org/10.1007/s12034-021-02610-3

61. Pressure induced structural, electronic and optical properties of wurtzite beryllium monoxide (w-BeO) from first-principle calculations.
Bimal Debnath, Manish Debbarma, Debankita Ghosh, Sayantika Chanda, Subhendu Das, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Solid State Communications (ELSEVIER) 342 (2022) 114571
https://doi.org/10.1016/j.ssc.2021.114571

62. First-principles calculations to investigate structural, mechanical, electronic, magnetic and thermoelectric properties of Ba_2CaMO_6 (M=Re, Os) cubic double perovskites
Subhendu Das, Manish Debbarma, Debankita Ghosh, Sayantika Chanda, Bimal Debnath, Rahul Bhattacharjee, **Surya Chattopadhyaya***
Physica B: Physics of Condensed Matter (ELSEVIER) 626 (2022) 413554.
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63. Tuning of optoelectronic and transport properties of zinc-blend magnesium chalcogenides through doping of Hg atom(s): The mBJ-GGA+U based first-principle calculations
Manish Debbarma, Debankita Ghosh, Sayantika Chanda, Bimal Debnath, **Surya Chattopadhyaya***
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64. First-principles calculations to investigate transformation of optically inactive zinc-blend beryllium chalcogenides to optically active semiconductor alloys through doping of Hg atom(s)
Manish Debbarma, Debankita Ghosh, **Surya Chattopadhyaya***
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65. Density functional study of structural and optoelectronic properties of wurtzite $Mg_xZn_{1-x}Te$ ternary alloys
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66. Theoretical investigation of magnesium compositional variation of structural and optoelectronic properties of wurtzite $Mg_xZn_{1-x}Se$ ternary alloys through first-principle calculations
Utpal Sarkar, Manish Debbarma, Debankita Ghosh, **Surya Chattopadhyaya***
Pramana-Journal of Physics (SPRINGER), In Press (2022).

Project:

Title of the Project	Awarding Agency	Period	Amount Sanctioned	Ongoing/ Completed
Quantum Mechanical Studies of the Electronic States of Oxides and Sulfides of Selenium and Tellurium	UGC, Govt. of India	01.04.2007-31.03.2010	Rs. 4,41,000/-	Completed

Seminar & Conference attended/organized

Sl. No.	Name of the Conference / Seminar with date	Organized by	National / International	Presented Paper/ Delivered Invited lecture
1	VI-th National Conference of the Physics Academy of the NORTH – EAST (PANE) (3-4th April, 2009)	Department of Physics, Tripura University	National	Presented Paper (Poster Presentation)
2	First International Conference on Materials Science (ICMS-2013) 21-23 February, 2013	Department of Physics, Tripura University	International	Presented Paper (Poster Presentation)
3	National Conference on Recent Trends of Research in Physics (NCRTRP-2015) 23-24 July, 2015	Department of Physics, Women's College, Agartala, Tripura.	National	Invited Lecture
4	UGC Sponsored National Seminar on "Recent Trend of Research in Chemistry - A new Horizon of Hopes". 08-09 August, 2015	Department of Chemistry, Women's College, Agartala, Tripura.	National	Presented Paper (Oral Presentation)
5	National Seminar on Recent Trends on Material Science. 01 March, 2016	Department of Chemistry, D.D.M. College, Khowai, Tripura.	National	Presented Paper (Oral Presentation)
6	UGC Sponsored National Seminar on "Chemistry Today and Tomorrow For Better Future". 05-06 August, 2016	Department of Chemistry, D.D.M. College, Khowai, Tripura.	National level	Presented Paper (Oral Presentation)
7	Second International Conference on Materials Science (ICMS-2017) 16-18 February, 2017	Department of Physics, Tripura University	International	Presented Paper (Poster Presentation)
8	Third International Conference on Materials Science (ICMS-2017) 04-06 March, 2020	Department of Physics, Tripura University	International	Presented Paper (Poster Presentation)
9	XII-th National Conference of the Physics Academy of the NORTH – EAST (PANE) (3-4th April, 2009)	Department of Physics, Tripura University	National	Presented Paper (Poster Presentation)