Dr. BIMAL KUMAR SARKAR

M.Sc. (Jadavpur University, India), AMIE (Electrical Engineering), Ph.D. (IACS, India), Postdoc (Taiwan, USA)

(1) Visiting Professor, SAV, Slovakia, (2) Visiting Scientist Max-Planck-Institut für Eisenforschung GmbH (MPIE), Germany

Research Profile
ORCID: 0000-0002-0168-2491
Scopus Id: 55326637400
Google Scholar: Total Citation 3144, h-index: 21; i10-index: 40
Personal Page

Research Project
Completed **FOUR** projects.
GoI Funding:2; Non-GoI: 2 (Detail in RESEARCH & DEVELOPMENT Table)
E-mail: bksarkar@outlook.in, Mob: 91-9910843342

PROFESSIONAL EXPERIENCE:

Regular Position

Professor and Dean (Science), Director (Planning), Adamas University, India	2018 - present
Professor & Dean, Galgotias University, Gr. Noida, India	2016 - 2018
Professor & Dean (Research), Galgotias University, Gr. Noida, India	2012 - 2016
Professor, Dept. of Physics, VIT University, Vellore, India	2009 - 2012
Professor, Dept. of Physics, Sanjay Inst.-U. P. Tech. Univ., India	2008 - 2009
Postdoctor, Dept. of Chem., Nat. Sun Yat-Sen Univ., Taiwan	2005 - 2008
Controller, CESC, Kolkata	1987 - 2005

Visiting / Short time Position

Controller of Examinations, Murshidabad University, West Bengal	2022
Visiting Professor, Brno University of Technology, Czech Republic (One month yearly)	2022 - 2023
Visiting Professor, Institute of Materials, Slovak Univ Tech, Slovakia (One month yearly)	2015 - 2018
Visiting Professor, Slovak Academy of Science, Slovakia (Two months)	2019
Visiting Scientist, Max-Planck-Institut für Eisenforschung GmbH (MPIE), Germany	2014
Visiting Professor, Nat. Sun Yat-sen Univ., Taiwan	2010
Visiting Scientist, Dept. of Chem., Nat. Sun Yat-Sen Univ., Taiwan	2008/09
Visiting Dept. of Chem. & Bio Chem., Uni. California at LA, USA	2008

UNIVERSITY / ACADEMIC RESPONSIBILITIES:
1. Academic affairs (Examination), Adamas University
2. Director, Adamas University
3. Dean, School of Basic and Applied Sciences, Adamas University
4. Member, Governing Board, Adamas University
5. Coordinator, NAAC, Adamas University
6. Coordinator, Research, Adamas University
7. Member, Academic Council, Adamas University
8. Member Secretary, Digital Media, Adamas University
9. Chairman, University Student Grievance Redressal Committee, Adamas University
10. Member, IQAC, Adamas University
11. Dean, School of Basic & Applied Science, Galgotias University
12. Dean Research, Galgotias University
13. Programme Chair of M.Sc.-Physics, Galgotias University
14. Centre Superintendent, COE Office, Galgotias University
15. Editor-in-Chief, Int. J. Engg. & Allied Sci., GU
16. Chair, Board of Studies, Physics – Galgotias University
17. Member, Board of Research, Galgotias University
18. Member, IQAC, Galgotias University
19. Chair, Board of Studies, Physics – VIT University
20. ABET, NAAC, VIT University

1. "Entropy study to monitor the complexity and health of a forest ecosystem", Brno University of Technology, Czech Republic, October 25, 2024. (**Invited Talk**)
2. "Entropy to understand the complexity and diversity of forest ecosystems", Technical University in Zvolen, Slovakia, October 23, 2024. (**Invited Talk**)
3. "Temperature dependence of elastic constants for ionic solids", Thermophysics2023, Dalešice, Czech Republic, October 3-5, 2023. (**Invited Speech**)
4. "Topological entropy calculations on the molecular sequences", Thermophysics2022, Dalešice, Czech Republic, October 4-6, 2022. (**Invited Speech**)
5. "DFT Calculations of Thermo-Mechanical Properties Of Be-Chalcogenides", Thermophysics2021, Dalešice, Czech Republic, September 7-9, 2021. (**Keynote Speech**)
6. "Photoacoustic Spectroscopy: A tool for Optical Properties Study", Thermophysics2020, Smolenice Castle, Slovak Republic, September 7-9, 2020. (**Keynote Speech**)
7. "Zr-Alloys at high temperature and pressure", Institute of Physics, Slovak Academy of Sciences, Bratislava, October 29, 2019. (**Invited Speech**)
8. "Pattern recognition analysis to explore molecular sequence", ICEMP 2018, Prague, June 15-18, 2018. (**Keynote Speech & Chairing**)
9. "Photoacoustic Spectroscopic Application for the Properties of Solids", NAA2017, Bangkok, January 3-5, 2017. (**Invited Speech & Chairing**)
10. "The study of the thermal and optical properties of smart materials: An application of Photoacoustic Spectroscopy", ICAEM2016, Jupiter Constanta, Romania, June 29-July 2, 2016. (**Keynote Speech & Chairing**)
11. "Canonical Correlation Analysis in pattern recognition: Application to HIV integration site", ICEMP 2015, Kuala Lumpur, June 11-12, 2015. (**Keynote Speech & Chairing**)
12. "Photoacoustic Spectroscopy for the investigation of thermal and optical properties of solids", New Advances in Acoustics (NAA2015), Shanghai, China. January 31 to February 2, 2015.
13. "Computational simulation of materials properties", ICEMP 2014, Hong Kong, June 14-15, 2014. (**Keynote Speech & Chairing**)
14. "Application of DFT in Material Properties Calculation", ICEMP 2013, Colombo, June 15-16, 2013. (**Keynote Speech & Chairing**)
15. "Photoacoustic Spectroscopy: A tool for the investigation of thermal and optical properties of solids", Czech Technical University, Prague, Czech Republic, Nov. 3, 2011. (**Keynote Speech & Chairing**)
16. "Diluted Magnetic Semiconductors", VIT University, Vellore, India, March 11, 2010.
17. "Progress of Nuclear Magnetic Resonance Micro-imaging: Methodologies and Applications", LNM Institute of Information Technology, Jaypur, India, Feb. 6-7, 2010. (**Keynote Speech**)
18. "Anisotropic Diffusion: a tool for the determination of tissue architecture deformation" CMC, Vellore, India, Oct. 9, 2009.
19. "Methodology and Application of Diffusion Tensor Imaging", Nuclear & Medical Physics Department, VIT University, Vellore, India, Sept. 12, 2009.
20. "Some Recent Progress of Nuclear Magnetic Resonance Micro-imaging", National Conference on Recent Advances on Solid State Materials & Devices (NCRA 2008., Mathura, India, Sept. 4-6, 2008. (**Keynote Speech & Chairing**)
21. "Development of Nuclear magnetic Resonance Micro-imaging and Its Applications in the Investigations of Micro-structure and Dynamics in Plant Seeds" First Cross-Strait Magnetic Resonance Conference, Hsinchu, Taiwan, Oct. 10-12, 2007.
22. "Progress of Magnetic Resonance Microimaging", Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan, December 3, 2006.
23. "Principle of Diffusion Tensor Imaging and MRI", Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan, Oct 23, 2006.
24. "Thermal and optical properties of Diluted Magnetic Semiconductors", Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan, July 2, 2005.
25. "Optimization of arresting fly ash in electro-precipitator", OM Institute, CESC, Calcutta, India, Dec 21, 2004.

MEMBER IN SCIENTIFIC SOCIETY

- Indian Association for the Cultivation of Science, Kolkata, India.
- Indian Statistical Institute, Kolkata, India.
- National Magnetic Resonance Society, IISc., Bangalore, India.
- International Society of Magnetic Resonance, ISMAR., USA.
- Assoc. of Medical Physicists of India.
- Int. Thermophysics, Central Europe.
- International Association of Computer Science and Information Technology (IACSIT), Singapore.
- Indian Science Congress.
- Asia-Pacific Chemical, Biological & Environmental Engineering Society (APCBEES)

AWARDS

- Research 2010, VIT University
- DST travel recipient 2010
- DST travel recipient 2014
- PAEU Fellowship, NSC, Taiwan 2010
- NSP Fellowship, Slovak Republic 2015
- Distinguished Reviewer in Elsevier Journals, 2015
- NSP Fellowship, Slovak Republic 2017
- NSP Fellowship, Slovak Republic 2018
- SAIA, European Research Fellowship, 2019

RESEARCH INTEREST:

Condensed matter and Biophysics

Condensed matter: Ab initio study of the structural, lattice dynamics, electronic, elastic, dielectric, optical properties of solids based on density functional theory (DFT) is performed to study the structural and electronic properties of solids. The thermodynamics properties including the phonon contribution are studied.

Biophysics: Computational information theory is applied for the investigation of network architecture of genome controlled signal transduction circuit. DNA dynamics is investigated based on probabilistic statistics and entropy calculation.

Research Highlights:

- PAE Fellowship, Taiwan, Enhancement of Micro-MRI resolution.
  J. Agric. Food Chem. 2009, 57, 18, 8213–8219.
- Academic Excellence Program, Taiwan, Application of MRS in detection of Biomarker.
  Front Biosci Landmark 2014, 19, 1186-201
- Study of phonon dispersion, lattice dynamics based on Density Functional Theory.
  Physica Scripta, 2014, 89 (7), 075704.
- NSP European Fellowship, Slovakia, Structure, Mechanical and Thermal Properties of Zr-Al-Nb Alloy.
  TMS 2015 144th Annual Meeting & Exhibition, 713-719.
- SAIA Research Fellowship, Slovak Academy of Science. Investigation of Heat Transfer in the Porous Materials.
- Molecular sequence study based on bio-inspired Electronic Filter.
  nature Scientific reports, 2021, 11 (13701), 1-12.

PUBLICATIONS
Google Citation
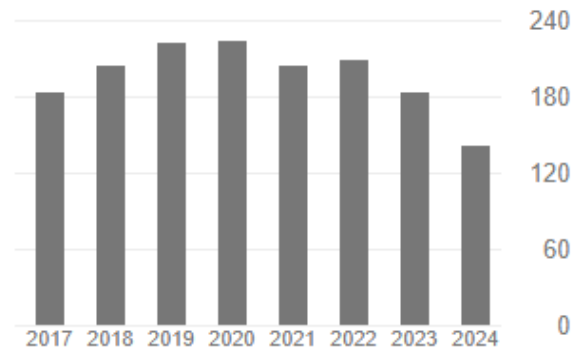
LIST OF PUBLICATIONS (Last 15 Years):

Journal papers:
2023

"Entropy-Driven, Integrative Bioinformatics Approaches Reveal the Recent Transmission of the Monkeypox Virus from Nigeria to Multiple Non-African Countries", Sarkar, B.K., Bhattacharya, M., Agoramoorthy, G. et al., *Mol Biotechnol* (2023). https://doi.org/10.1007/s12033-023-00889-7

"Topological entropy calculations on the molecular sequences", A Sarkar, BK Sarkar, O Zmeskal, *AIP Conf. Proc.* 2894, 020017 (2023)

2022

"Determination of growth exponent for percolating clusters of various lattices", PSD Prasadh, A Arulgnanam, BK Sarkar, B Saravanakumar, *J. Physics: Conf. Series*, 2349, 012011 (2022).

"DFT calculations of thermo-mechanical properties of Be-chalcogenides", B K Sarkar, *AIP Conf. Proc.*, 2488, 020024 (2022).

2021

"Determination of k-mer density in a DNA sequence and subsequent cluster formation algorithm based on the application of electronic filter", B K Sarkar, C Chakraborty, A R Sharma, G Sharma, J-E Lee, *nature Scientific Reports* 11, 13701 (2021).

"Understanding the Molecular Evolution of tiger diversity through DNA barcoding marker ND4 and NADH dehydrogenase complex using computational biology", B K Sarkar, C Chakraborty, A R Sharma, G Sharma, J-E Lee, *Genes and Genomics* 43, 759–773 (2021).

"Entropy of DNA sequences as similarity index for various SARS-CoV-2 virus strains", S. Biswas, B.K. Sarkar, In **Advances in Medical Physics and Healthcare Engineering**, Springer, pp.533-543 (2021).

"Entropy Based Biological Sequence Study", In **Entropy and Exergy in Renewable Energy**, Bimal Kumar Sarkar, pp. 1-8, (2021). DOI: 10.5772/intechopen.96615.

2020

Bimal Kumar Sarkar and Sukriti Sarkar Photoacoustic spectroscopy: A tool for optical properties study *AIP Proceedings* 2305, 020017, (2020)

Paramita Saha, Bimal Kumar Sarkar Entropy based analysis of Genetic Information *J. Physics:IOP Series,* 1579 (1), 012003, (2020)

2018

"The novel strategies for next-generation cancer treatment: miRNA combined with chemotherapeutic agents for the treatment of cancer": C Chakraborty, A R Sharma, G Sharma, J-E Lee, B K Sarkar, S-S Lee, *Oncotarge* 9 (2018) 10164-10174.

2017

"Ab Initio Study of Electronic, Structural, Thermal and Mechanical Characterization of Cadmium Chalcogenides": PS, Devi Prasadh; Sarkar, BK; *Mechanics, Materials Science & Engineering Journal*, 9 (2017) 9-11.

2016

Deviprasadh P S, Madhuri W., B. K. Sarkar,"Photoacoustic spectroscopic study of optical properties of Cu2GeTe3 in temperature range from 70 to 300 K", *Int J. Thermophysics* 37:50 (2016) 1-9.

2015

"DNA pattern recognition using canonical correlation algorithm",B. K. Sarkar, C. Chakraborty, *J. Biosciences*, 40, (2015), 709.

"Principal Component based method for whole genome phylogenetic analysis without alignment: Application to HEV genotype", Subrata Sahana, Sanjoy Das, Bimal Kumar Sarkar, *IEEE Computing, Communication &Automation* ICCCA, (2015) 984 - 989.

"First-Principles Phase Stability Calculations of Zr3Al1-xNbx Alloys with L12, and DOa Structures",Bimal Kumar Sarkar, Ajay Sing Verma, Deviprasadh P S, *TMS Annual Meeting*, 2015, s. 713-719.

2014

"Novel biomarker for prostate cancer diagnosis by MRS": Bimal Kumar Sarkar, Chiranjib Chakraborty, Ashish Ranjan Sharma, Kee-Jeong Bae, Garima Sharma, George Priya Doss, Debnarayan Dutta , Shangwu Ding, Bilguun Ganbold, Ju-Suk Nam, Sang-Soo Lee, *Frontiers in Bioscienc*e 19 (2014) 1186.

"Barrier–Cluster–Heating Model and Photoinduced Phenomena in Chalcogenide Glasses": Ivan Banik, Jozefa Lukovičová, Peter Šín, Bimal Kumar Sarkar, *AIP Conf. Proc.* 1634 (2014) 100.

"Evaluating structural, optical & electrical characterization of zinc chalcogenides – FP–LAPW+ l0 method": Deviprasadh P S, B. K. Sarkar, Madhuri W., Int. J. Sci. Engg. Appl. Special Issue NCRTAM ISSN-2319-7560 (2014) 29.

"Optical Properties of Cd1-xZnxSe from Density Functional Theory": Bimal Kumar Sarkar, Ajay Singh Verma, Gabriela Pavlendova, Ivan Banik, Proc. TMS 2014 (2014).

"Ab-Initio Calculations of Structural, Electronic, and Optical Properties of Cd1–XMnxTe": B. K. Sarkar, I*nt. J. Appl. Phys. Math.,* 4, (2014), 76.

"First-principles calculations of structure, phonon and thermal properties of ZnX (X = S, Se,Te) chalcogenides": B. K. Sarkar, A. S. Verma, S. Sharma, S. K. Kundu, *Phys. Scr.* 89 (2014) 075704.

2013

"Compensation effect in the amorphous hydrogenated silicon from point of view of the barrier-cluster model": Ivan Baník, Jozefa Lukovičová, Gabriela Pavlendová, Bimal Kumar Sarkar, *Act. Electrotechnica et Informatica,* 13 (2013) 26.

"Support Vector Machine and Relevance Vector Machine for Prediction of Alumina and Pore Volume Fraction in Bioceramics": K G S Gopinath, Soumen Pal, Pijush Samui and Bimal Kumar Sarkar, *Int. J. Appl. Ceram. Technol.,* 10 (2013) E240–E246.

"Mapping the Structural Topology of IRS Family Cascades Through Computational Biology": Chiranjib Chakraborty, C. George Priya Doss, Sanghamitra Bandyopadhyay, Bimal Kumar Sarkar, S. A. Syed Haneef, *Cell Biochem Biophys* 67 (2013) 1319.

2012

"Information processing in network architecture of genome controlled signal transduction circuit - A proposed theoretical explanation": Sarkar BK, Chakraborty C, Patel P, Agoramoorthy G, *Theoretical biology forum* 105 (2012) 67.

"Ab initio calculation of structure, lattice dynamics and thermal properties of zinc-blende structure ZnX (X = S, Se,Te)": B. K. Sarkar, A. S. Verma, S. K. Kundu, Sheetal Sharma, V. K. Jindal, Submitted in *Phys. Scr. (*2012).

"Dielectric constants of zinc-blende semiconductors": B K Sarkar, A S Verma, Naresh Pal, R Bhandari and V K Jindal, *Phys. Scr.* 85 (2012) 015705.

"Elastic properties of chalcopyrite structured solids":, A. S. Verma, Sheetal Sharma, R. Bhandari, B. K. Sarkar, V. K. Jindal, *Mat. Chem. Phys.* 132 (2012) 416.

2011

"FP-LAPW + lo calculations for the structural, electronic, optical and mechanical properties of ZnX (X = S, Se and Te)": B. K. Sarkar, Sheetal Sharma, A. S. Verma, and V. K. Jindal, *AIP Conf. Proc.* 1447 (2011) 849. doi:http://dx.doi.org/10.1063/1.4710269, (ISBN 978-0-7354- 0963-7)

"First principles study on the elastic and electronic properties of CdX (X = S, Se and Te)": Sheetal Sharma, Ajay Singh Verma, Bimal Kumar Sarkar, Rajiv Bhandari and Vijay Kumar Jindal, *AIP conf. P*roc 1394 (2011) 229. (ISBN 978-0-7354-0963-7)

"Electronic and mechanical properties of ZnX (X = S, Se andTe) – An ab initio study": Ajay Singh Verma, Sheetal Sharma, Bimal Kumar Sarkar and Vijay Kumar Jindal, *AIP conf. Proc* 1394 (2011) 237. (ISBN 978-0-7354-0963-7)

"Temperature induced band gap shrinkage in Cu2GeSe3: Role of Electron-phonon interaction": Bimal Kumar Sarkar, Ajay Singh Verma, P. S. Deviprasad, *Physica B* 406 (2011), 2847.

"Models for lattice thermal expansion and thermal conductivity for ternary (ANB2+NC27-N) tetrahedral semiconductors": Ajay Singh Verma, Bimal Kumar Sarkar, Sheetal Sharma1, Rajiv Bhandari and Vijay Kumar Jindal, *Mat. Chem. Phys*., 127 (2011), 74.

2010

"Cohesive energy of zinc blende (AIIIBV and AIIBVI) structured solids": A. S. Verma, B. K. Sarkar and V. K. Jindal, *Pramana J Physics*, 74 (2010), 851.

"Inherent properties of binary tetrahedral semiconductors": A. S. Verma, B. K. Sarkar, V.K. Jindal, Physica B, 405 (2010), 1737.

"Thermal and optical properties of Zn1-xMnxTe diluted magnetic semiconductor studied by photoacoustic spectroscopic method": B. K. Sarkar, A. S. Verma, R. C. Gupta and K. Singh, *Int. J. Thermophysics*, 31 (2010), 620.

2009

"Temperature dependence of elastic constants for ionic solids": Bimal Kumar Sarkar, Ajay Singh Verma, Rajesh Chandra Gupta, *Physica B*, 404 (2009), 4106.

"Variation of Local Environment and Dynamics of Water and Oil Molecules during Germination of Sesamum indicum Seed: A Nuclear Magnetic Resonance Spectroscopic Investigation": Bimal Kumar Sarkar, Wei-Yuan Yang, Zhen Wu, Huiru Tang, and Shangwu Ding, *J. Agr. Food Chem.* 57 (2009), 8213.

"Micro-magnetic resonance imaging (micro-MRI) study on the sepsis effected eyeball of zebrafish": Bimal Kumar Sarkar, Wu Zen, Shangwu Ding, C. H. Hsu, Z.H. Wen, C. S. Lin, C. Chakraborty, *Nature Prec.* (2009) On-line, http://hdl.handle.net/10101/npre.2008.2694.1.

Conference Papers:

37. "Entropy of DNA Sequences as Similarity Index for Various SARS-CoV-2 Virus Strains": Satarupa Biswas and Bimal Kumar Sarkar, AMPHE2020, Adamas University, September 25-26, 2020.

36. "The study of the thermal and optical properties of smart materials: An application of Photoacoustic Spectroscopy": Bimal Kumar Sarkar, ICAEM2016, Jupiter Constanta, Romania, June29- July 2, 2016.

35. "First-Principles Phase Stability Calculations of Zr3Al1-xNbx Alloys with L12, and DOa Structures": Bimal Kumar Sarkar, Ajay Sing Verma, Deviprasadh P S, TMS2015, Orlando, Florida, 15-19 March, 2015.

34. "Thermal and optical properties of Cd1-xZnxSe semiconductor from photoacoustic measurement": B. K. Sarkar, G. Pavlendova, I. BANIK, 3Deviprasadh PS, Thermophysics 2014, Podkylava, Slovakia, 8- 10 Oct, 2014.

33. "Thermo-mechanical properties of Be-chalcogenides from density functional theory": B. K. Sarkar, G. Pavlendova, I. BANIK, A. S. Verma, Thermophysics 2013, Podkylava, Slovakia, 13- 15 Nov, 2013.

32. "Electronic and Thermal properties of Zinc Chalcogenides based on Density Function Theory": B. K. Sarkar, G. Pavlendova, I. Banik, A. S. Verma, Thermophysics 2012, Podkylava, Slovakia, Oct. 31- Nov 2, 2012.

31. "Electrical conductivity in the amorphous hydrogenated silicon and Meyer-Neldel rule": I. Banik, J. Lukovičová, G. Pavlendová, B. K. Sarkar, Proc. Scientific Conference Physics of Materials 2012, Košice, Slovakia, 17-19 Oct. 2012.

30. "Temperature dependent optical bandgap in Cu2GeS3 by photoacoustic spectroscopy": B. K. Sarkar, A. S. Verma, Proc. the 3rd International Conference on the Physics of Optical Materials and Devices, 3rd - 6th September 2012, Belgrade.

29. "Compensation Effect in Kinetics of Crystallization and Catalyzis in Disordered Materials", Ivan Banik, Jozefa Lukovicova, Gabriela Pavlendova, Bimal K. Sarkar, Proc. International Conference on Recent Trends in Advanced Materials, ICRAM-2012, Vellore, India, 20-22, February 2012.

28. "Micro Magnetic Resonance Imaging Technique for the investigation of water diffusion in the plant vascular bundles", B. K. Sarkar, C Anu Radha and V. Ramasubramanian, Proc. 18th National Magnetic Resonance Society, NMRS 2012, IISc., Bangalore, India, February 5-8, 2012.

27. "Photoacoustic Spectroscopy: A tool for the investigation of thermal and optical properties of solids", B. K. Sarkar, Deviprasadh P S, A. S. Verma, Sheetal Sharma, V. K. Jindal, Proc. Thermophysics 2011, Brno, Czech Republic, Nov. 2-4, 2011.

26. "Thermo-elastic properties of nonmaterials at high temperature: A finite strain approach": Deviprasad P S, A. S. Verma and B. K. Sarkar, 12th international symposium on physics of materials (ISPMA 12), September 4 - 8, 2011, Prague, Czech Republic.

25. "NMR characterization of metabolites in prostate adenocarcinoma": Sarkar B K and Chakraborty C, Proc. International Conference on Medical Physics in Radiation Oncology and Imaging (ICMPROI-2011) 11-13 March 2011, Dhaka, Bangladesh.

24. "Magnetic resonance spectroscopic estimation of metabolite biomarker for prostate cancer characterization": Bimal Kumar Sarkar and Kalai Selvan N, Proc. Magnetic Moments in Central Europe (MMCE 2011), March 16 – 18, 2011, Tatranská Lomnica, Sovakia.

23. "Photoacoustic spectroscopic investigation of temperature dependence of optical absorption in Cu2GeSe3": B. K Sarkar and A. S. Verma, Proc. Thermophysics 2010, 3-5 November, 2010, Brno University of Technology, Valtice, Czech Republic.

22. "Photoacoustic investigation of bandgap and band-edge effective mass of Zn1-xMnxTe magnetic semiconductor": B. K. Sarkar, R. L. Hota and A. S. Verma, Proc. 23rd General Conference of the Condensed Matter Division of the European Physical Society, 30 August – 3 September 2010, Warsaw, Poland.

21. "Magnetization in IV-VI based DMS": B. K. Sarkar, R. L. Hota, Proc. 14th National Seminar on Crystal Growth (in association with Indian Association for Crystal Growth), 2010, Vellore, India.

20. "NMR study of water uptake and lipid consumption during germination of plant seed": B. K. Sarkar, S. Ding, Proc. National Symposium on Science and Technology and the Young, 2009, Kolkata, India.

19. "Effects of doping on optical band gap of Zn1-xMnxTe Magnetic Semiconductors": B. K. Sarkar, R. C. Gupta, S. K. Choudhary, A. S. Verma, Proc. The International Conference on Magnetism - ICM 2009, Karlsruhe, Germany.

18. "NMR spectroscopic investigation of water uptake and oil mobilization during Sesamum indicum seed germination": B. K. Sarkar, S. Ding, Proc. 23rd International Conference on Magnetic Resonance in Biological Systems (XXIII ICMRBS), 2008, San Diego, California, USA.

17. "Investigation of water diffusion in the vascular bundles in the stem of sesame plant by Micro Magnetic Resonance Imaging": B. K. Sarkar, Z. Wu, S. Ding, Proc. 49th Experimental Nuclear Magnetic Resonance Conference (49th ENC), 2008, Pacific Grove, California, USA.

16. "NMR Investigation of Oil Molecules Dynamics and Water uptake during the Germination of Plant Seed": B. K. Sarkar, W-Y Yang, S. Ding, Proc. National Conference on Recent Advances on Solid State Materials & Devices (NCRA 2008), Mathura, India.

15. "Microscopic magnetic resonance imaging investigation on the Induction of hyperglycemia in zebrafish": B. K. Sarkar, Z. Wu, S. Ding, 14th National Magnetic Resonance Society Meeting, NMRS-2008, Delhi, India.

14. "Development of Nuclear magnetic Resonance Micro-imaging and Its Applications in the Investigations of Micro-structure and Dynamics in Plant Seeds": Yang WY, Shi YR, Sarkar B K, Wu Z, Ding S. Proceeding of First Cross-Strait Magnetic Resonance Conference, 2007, Hsinchu, Taiwan.

13. "Probing the water transport and physiology of plant cell by micro-MRI": Bimal Kumar Sarkar, Zhen Wu, Shangwu Ding, 16th Triennial Conference for the International Society of Magnetic Resonance, ISMAR, 2007, Kenting, Taiwan.

12. "Magnetic Resonance Micro-Imaging Studies of the Sepsis Effected Eyeball of Zebra Fish": Bimal Kumar Sarkar, Zhen Wu, Shangwu Ding, 48th Experimental Nuclear Magnetic Resonance Conference (48th ENC), 2007, Daytona, Florida, USA.

11. "Diffusion Tensor Weighted Microscopic NMR Imaging": B. K. Sarkar, Z. Wu, S. Ding, Proceeding of Chemical Society Located in Taipei 2005, Taiwan, Nov. 19-20, 2005, p.223.

10. "Photoacoustic measuring technique for the investigation of thermal properties of high Tc superconducting materials": S. Sarkar, Bimal Kumar Sarkar, Proc. European Conference on Thermophysical Properties (ECTP 2005), Bratislava, Slovakia.

9. "Er-doped Gallium Nitride thin film as hybrid light emitting devices": B. K. Sarkar, S. Chatterjee, B. K. Chaudhuri Proc. 6th International Conference on Nitride Semiconductors (ICNS 6), Bremen, Germany, 2005.

8. "Effect of annealing on the magnetic properties of III-V based ferromagnetic GaMnAs semiconductor": B. K. Sarkar, B. K. Chaudhuri, Proc. 3rd International Conference on Materials for Advanced Technologies (ICMAT 2005), Singapore.

7. "Effect of Mn doping on the optical band gap of Zn-Mn-Se diluted magnetic semiconductor": S. chatterjee, B. K. Sarkar, B. K. Chaudhuri, Condensed Matter and Materials Physics Conference (CMMP04), April 2004, University of Warwick, UK.

6. "Carrier-induced ferromagnetism in the nitrogen doped diluted magnetic semiconductor Zn1−xMnxSe": B. K. Sarkar, S. Sarkar, The 20th General Conference of the Condensed Matter Division of the European Physical Society, 2004, the Prague Congress Center, Prague, Czech Republic.

5. "Frequency dependent dielectric behavior of polyaniline-fly ash composites": B. K. Sarkar, S. Sarkar, B. K. Chaudhuri,The 20th General Conference of the Condensed Matter Division of the European Physical Society, 2004, the Prague Congress Center, Prague, Czech Republic.

4. "The effect of Be substitution on the optical response of Zn1-xBexSe Semiconductors": B. K. Sarkar, S. Sarkar, B. K. Chaudhuri, 2nd International Conference on Structure, Processing and Properties of Materials, BUET, Dhaka, Bangladesh, 2004.

3. "Optical absorption of Zn1-XMnXSe ($0 \leq X \leq 0.5$) type diluted semiconductor": B. K. Sarkar, B. K. Chaudhuri, Material Congress, March, 2004, Carlton House Terrace, London, UK.

2. "Photoacoustic spectroscopic study of optical band gap of Zn1-xBexSe Semiconductors": 15th symposium on Thermophysical Properties, B. K. Sarkar, B. K. Chaudhuri, National Institute of Standards and Technology, Colorado, USA, June, 2003.

1. "Photoacoustic study of the thermal properties of the high TC superconductor (Bi,Pb)-Sr-Ca-Cu-O": B. K. Sarkar, K. chaudhuri, National Conference on Thermophysical Properties (NCTP), March, 1999, Physics department, Guahati university, Assam, India

Front page of some papers are given in the next page.

ORIGINAL PAPER

Entropy-Driven, Integrative Bioinformatics Approaches Reveal the Recent Transmission of the Monkeypox Virus from Nigeria to Multiple Non-African Countries

Bimal Kumar Sarkar[1] · Manojit Bhattacharya[2] · Govindasamy Agoramoorthy[3] · Kuldeep Dhama[4] · Chiranjib Chakraborty[5]

Abstract

Monkeypox virus (mpox) has currently affected multiple countries around the globe. This study aims to analyze how the virus spread globally. The study uses entropy-driven bioinformatics in five directions to analyze the 60 full-length complete genomes of mpox. We analyzed the topological entropy distribution of the genomes, principal component analysis (PCA), the dissimilarity matrix, entropy-driven phylogenetics, and genome clustering. The topological entropy distribution showed genome positional entropy. We found five clusters of the mpox genomes through the two PCA, while the three PCA eluci-dated the clustering events in 3D space. The clustering of genomes was further confirmed through the dissimilarity matrix and phylogenetic analysis which showed the bigger size of Cluster 1 and size similarity between Clusters 2 and 4 as well as Clusters 3 and 5. It corroborated with the phylogenetics of the genomes, where Cluster 1 showed clear segregation from the other four clusters. Finally, the study concluded that the spreading of the mpox is likely to have originated from African countries to the rest of the non-African countries. Overall, the spreading and distribution of the mpox will shed light on its evolution and pathogenicity of the mpox and help to adopt preventive measures to stop the spreading of the virus.

Graphical Abstract
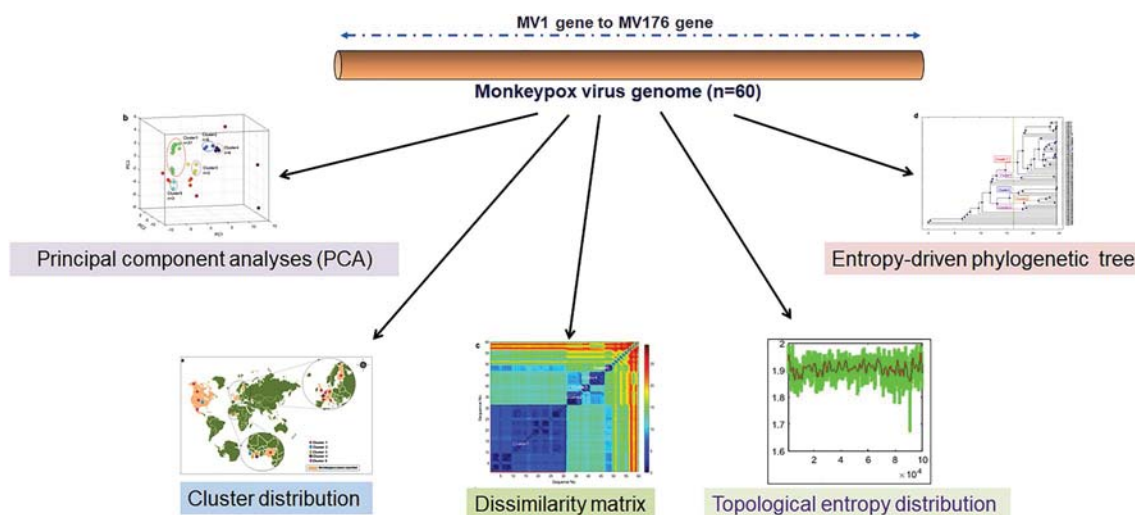
Keywords Monkeypox virus · Entropy · Bioinformatics · Africa

Abbreviations
Mpox   Monkeypox
PCA   Principal component analysis

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Determination of k-mer density in a DNA sequence and subsequent cluster formation algorithm based on the application of electronic filter

Bimal Kumar Sarkar[1,6], Ashish Ranjan Sharma[2,6], Manojit Bhattacharya[3], Garima Sharma[4], Sang-Soo Lee[2✉] & Chiranjib Chakraborty[5✉]

We describe a novel algorithm for information recovery from DNA sequences by using a digital filter. This work proposes a three-part algorithm to decide the k-mer or q-gram word density. Employing a finite impulse response digital filter, one can calculate the sequence's k-mer or q-gram word density. Further principal component analysis is used on word density distribution to analyze the dissimilarity between sequences. A dissimilarity matrix is thus formed and shows the appearance of cluster formation. This cluster formation is constructed based on the alignment-free sequence method. Furthermore, the clusters are used to build phylogenetic relations. The cluster algorithm is in good agreement with alignment-based algorithms. The present algorithm is simple and requires less time for computation than other currently available algorithms. We tested the algorithm using beta hemoglobin coding sequences (HBB) of 10 different species and 18 primate mitochondria genome (mtDNA) sequences.

Over the last two decades, available DNA sequence data has grown exponentially. The understanding of the biological information and their implication with huge amount of DNA data has emphasized the crucial need for supportive sequencing methodologies. The development of cost-effective, efficient, and fast methods for sequence study is highly demanded. Substantial information for DNA sequence that put forward the arrangement of sequences variability indicates that the quantum of sequences that might have occurred throughout history is fewer in comparison to all possible sequences[1,2]. For example, considering 100 bp DNA sequence, one can construct as much as 4^{100} possible sequences. It demonstrates that only few of them thus exist in reality. The four letters A, C, G and T which denotes the four nucleotides, make the alphabetic sequence for coding genetic information. The genome sequences which consist of different gene can be readable by computer. Dealing with DNA sequence with computer becomes one of the prime domains in bioinformatics. It has vast application in data mining, comparative genomics, molecular phylogeny and genome annotation.

There are two types of methodology followed in sequence analysis-one is based on alignment and other is alignment free. In case of closely related sequence comparison, alignment-based methods are generally used. While dealing with divergent sequence it is better to use alignment free method[3–6]. On the other hand, alignment-based approach needs multiple or pairwise sequence alignments. Analyzing large datasets with an alignment-based method can surpass computational resources. Even sometimes, the combinatorics of genomic reorganisations makes the alignment of whole genomes quite difficult. A comparison of the alignment-based and alignment-free algorithm is given in Table 1.

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RESEARCH ARTICLE

Understanding the molecular evolution of tiger diversity through DNA barcoding marker ND4 and NADH dehydrogenase complex using computational biology

Chiranjib Chakraborty[1,2] · Ashish Ranjan Sharma[1] · Garima Sharma[3] · Manojit Bhattacharya[1] · Bidhan C. Patra[4] · Bimal Kumar Sarkar[5] · Saptarshi Banerjee[6] · Kankana Banerjee[6] · Sang-Soo Lee[1,7]

Abstract

Background Currently, Tigers (the top predator of an ecosystem) are on the list of endangered species. Thus the need is to understand the tiger's population genomics to design their conservation strategies.

Objective We analyzed the molecular evolution of tiger diversity using NADH dehydrogenase subunit 4 (ND4), a significant electron transport chain component.

Methods We have analyzed nucleotide composition and distribution pattern of ND genes, molecular evolution, evolutionary conservation pattern and conserved blocks of NADH, phylogenomics of ND4, and estimating species divergence, etc., using different bioinformatics tools and software, and MATLAB programming and computing environment.

Results The nucleotide composition and distribution pattern of ND genes in the tiger genome demonstrated an increase in the number of adenine (A) and a lower trend of A+T content in some place of the distribution analysis. However, the observed distributions were not significant ($P > 0.05$). Evolutionary conservation analysis showed three highly align blocks (186 to 198, 406 to 416, and 527 to 545). On mapping the molecular evolution of ND4 among model species ($n = 30$), we observed its presence in a broader range of species. ND4 based molecular evolution of tiger diversity and time divergence for a tiger (20 different other species) shows that genus *Panthera* originated more or less at a similar time.

Conclusions The nucleotide composition and nucleotide distribution pattern of tiger ND genes showed the evolutionary pattern and origin of tiger and *Panthera* lineage concerning the molecular clock, which will help to understand their adaptive evolution.

Keywords Tiger · NADH dehydrogenase subunits · DNA barcoding marker · NADH dehydrogenase subunit 4 (ND4) · Species divergence · Molecular clocks

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Chiranjib Chakraborty and Ashish Ranjan Sharma contributed equally to this work.

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Review

The novel strategies for next-generation cancer treatment: miRNA combined with chemotherapeutic agents for the treatment of cancer

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ABSTRACT

Medical practitioners are recommending combination therapy in cancer for its various advantages. Combination therapy increases the efficacy of treatment due to its synergistic effects in cancer treatment. In this post-genomic era, microRNAs (miRNAs) are receiving attention for their role in human disease and disease therapy. In this review, we discuss the combination of miRNAs and chemotherapeutic agents for cancer treatment. Moreover, we attempted to portray the role of miRNAs in cancer therapy; outline combination therapy, especially chemo-combination therapy, and discuss the basis for miRNA-based chemo-combination therapies and chemo-combination therapy with miRNA for cancer treatment.

INTRODUCTION

Since human genome sequencing and the advancement of the post-genomic era, a new wave of RNomics has been generated, and our understanding about small non-coding RNAs (ncRNAs) has grown exponentially [1, 2]. Among these ncRNAs, microRNAs (miRNAs) are receiving increasing attention because they regulate gene expression at the post-transcriptional level. miRNAs are non-protein-encoding RNAs that range in size from 19 to 25 nucleotides (nt). As for usual protein-coding mRNA, it has been noted that miRNAs are transcribed through RNA polymerase II. Then, they are spliced, capped and poly-adenylated, resulting in the primitive miRNA (pri-miRNA). Subsequently pri-miRNAs are processed through an endonuclease (RNase III endonuclease, called Drosha), generating the hairpin 'precursor' miRNAs. In animals, these 'precursor' miRNAs are ~70 nt long in the nucleus. However, in plants, the precursor miRNA length is longer at approximately ~100 nt in the nucleus [3]. Then, the hairpin precursor miRNAs bind to exportin-5 and RNA GTPase, which permits the transport of the molecules into the cytoplasm. The "precursor" miRNA is then processed into ~22 nt miRNA duplexes by Dicer [4]. miRNAs participate in several cellular functions, such as cell differentiation, cell cycle regulation and apoptosis [5]. miRNAs are important molecules with a vital role in human diseases and manages different cellular pathways in human diseases [6–8]. Chakraborty et al., described the occurrence of miRNAs that were linked with the regulation of key proteins related to insulin resistance and the insulin signaling pathway [9]. In another study, Chakraborty et al., described the occurrence and responsibility of miRNAs in the insulin signaling pathway and associated pancreatic cancer development [10]. The role of miRNAs in controlling MAPK signaling pathways in chronic myeloid leukemia has recently been reviewed [11]. Chakraborty et al., also reviewed miRNA controlled cancer stem cells that can help to understand

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Photoacoustic Spectroscopic Study of Optical Properties of Cu_2GeTe_3 in Temperature Range from 80 K to 300 K

P. S. Deviprasadh[1,2] · **W. Madhuri**[2] · **A. S. Verma**[3] · **B. K. Sarkar**[4]

Abstract We used photoacoustic spectroscopy to investigate the optical properties of Cu_2GeTe_3. The temperature dependence of the bandgap energy was evaluated from optical absorption spectra obtained in the photon energy range of 0.76 eV to 0.81 eV between 80 K and 300 K. We used the empirical and semi-empirical models of Varshni, Viña, and Pässler to describe the observed bandgap shrinkage in this compound. The Debye temperature and effective phonon temperature of the compound were estimated to be approximately 227.4 K and 151.6 K, respectively. Thus, the temperature dependence of the bandgap is mediated by acoustic phonons.

1 Introduction

Alexander Graham Bell discovered that if a solid sample kept in a cell which is irradiated with an intensity-modulated beam of light, sound is produced [1,2]. This phenomenon is known as the photoacoustic (PA) effect. In the experiment, the sample occupied a part of the cell and the remaining part was occupied by a gas (e.g., air). The PA effect is also observed for gas and liquid samples, where the sam-

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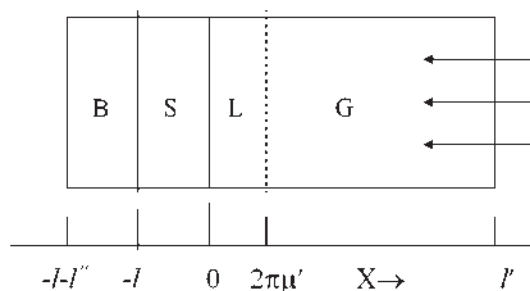4 Department of Physics, Galgotias University, Greater Noida 201308, India

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ple fills the whole container. Upon absorption of incident radiation, the internal energy levels of the sample are raised to excited states. During subsequent de-excitation, part or all of the absorbed photon energy is transformed into heat via non-radiative processes. When intensity-modulated light falls irradiates a solid sample, the heat production is periodic in nature. As a result, there is periodic heat flow from the interior of the sample to the surrounding gas. Periodic heat flow causes periodic pressure variations in the gas, which results in the production of acoustic signals. A microphone incorporated in the gas column can detect the acoustic signals.

Photoacoustic spectroscopy (PAS), which is essentially a combination of optical absorption spectroscopy and calorimetry, is a very sensitive tool for detecting small fluctuations in optical and thermal properties of a sample [3]. In the present study, we used the PAS technique to investigate the narrow optical bandgap shrinkage of the $A_2^I B^{IV} C_3^{VI}$-type ternary semiconducting compound, Cu_2GeTe_3. Owing to their small bandgap, such semiconductors have become very important materials in electro-optic applications in the IR region [4–9]. We used PAS [10] to study the optical absorption of Cu_2GeTe_3 at different temperatures.

2 Theoretical Model

According to Rosenzweig and Gersho (R–G theory) [11,12], the signal from a gas microphone PA cell depends on the acoustic pressure disturbance at the sample/gas interface and on the transport of this pressure disturbance through the gas to the microphone. The pressure fluctuation at the sample/gas interface caused by the periodic heat flow is modeled as an acoustic piston that is governed by thermal diffusion equations. Therefore, by solving the thermal diffusion equations, the periodic variation in temperature at the sample/gas interface can be obtained. A one-dimensional analysis of the production of a photoacoustic signal in a simple cylindrical cell is shown in Fig. 1. The cell has a diameter, D, and length, L. It is assumed that the length L is small compared with the wavelength of the acoustic signal, and the microphone (not shown in figure) detects the average pressure in the cell. The solid sample considered has the form of a disk with a diameter, D, and length, ℓ. The sample is mounted such that its back surface is in contact with a poor thermal conductor of thickness, ℓ''.

Fig. 1 Cross sectional view of a simple cylindrical PA cell

DNA pattern recognition using canonical correlation algorithm

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We performed canonical correlation analysis as an unsupervised statistical tool to describe related views of the same semantic object for identifying patterns. A pattern recognition technique based on canonical correlation analysis (CCA) was proposed for finding required genetic code in the DNA sequence. Two related but different objects were considered: one was a particular pattern, and other was test DNA sequence. CCA found correlations between two observations of the same semantic pattern and test sequence. It is concluded that the relationship possesses maximum value in the position where the pattern exists. As a case study, the potential of CCA was demonstrated on the sequence found from HIV-1 preferred integration sites. The subsequences on the left and right flanking from the integration site were considered as the two views, and statistically significant relationships were established between these two views to elucidate the viral preference as an important factor for the correlation.

1. Introduction

Progresses in genome sequencing technology enable scientists to search some common sequence elements in the DNA sequence. For example, DNA-binding proteins composed of DNA-binding domains are likely to bind related DNA sequences (Dickerson 1983; Pabo and Sauer 1984). Searching for functionally similar DNA sequences is very important to find some particular pattern in the sequence. In order to identify common patterns, several search approaches can be found in the literature. Hertz and Stormo (1999) modelled a succession of mechanisms to conclude alignments of multiple sequences. Based on the greedy algorithm they described log-likelihood scoring systems for searching alignments of functionally related sequences. Guha Thakurta and Stormo (2001) implemented Gibbs sampling method to explore subjective binding site patterns in DNA sequences. In Gibbs sampling method a stochastic variant of expectation maximization is determined (Lawrence *et al.* 1993; Neuwald *et al.* 1995) and a predetermined motif is substituted by another one that possesses a higher score, thus

permitting escape from local optima. An algorithm based on palindromic behaviour between the frequencies of bases was formulated to explore the integration sites in HIV-1 consensus sequences (Holman and Coffin 2005; Wu *et al.* 2005). But in such stochastic motif detection algorithm, it sometimes results in non-identical outputs in multiple runs of the simulation, keeping the input unchanged. Another drawback is that they are single modal techniques that can only deal with data from a single view. However, multimodal data from the semantic groups is prevalent in practice. Therefore, handling such multimodal data at the same time is a fundamental and practical problem. One effective method to address this issue is 'canonical correlation analysis' (CCA) (Hotelling 1936).

CCA compares two sets of multidimensional variables (in this case, a set of DNA sequence and a set of pattern) to examine the correlation between them (Hotelling 1936). CCA looks for correlated functions which are covariates of two different sets having some relation (Kettenring 1971; Johnson and Wichern 1992; Hardoon *et al.* 2004; Tenenhaus and Tenenhaus 2011). The attainability of such correlated

Keyword. Canonical correlation analysis; DNA sequence; pattern recognition

functions of two semantic sets is likely to persist due to a causal factor accountable for the correlation. CCA aims to discover the correlation between a linear combination of the variables in one set and another linear combination of the variables in the other set by projecting them onto a lower-dimensional space and maximum correlated (Kettenring 1971; Breiman and Friedman 1985; Yu *et al.* 2006; Iaci *et al.* 2010). The advantage of CCA is evident: First, it keeps the operative discriminant information of multiple modalities; secondly, it also removes the information redundancy to a certain limit. Thus, CCA has received more attentions in pattern recognition (Liang *et al.* 1995; Zhou and Shen 2009; Lei *et al.* 2010; Jing *et al.* 2011; Yuan *et al.* 2011). In this article, we describe an algorithm for recognizing a pattern in DNA sequence based on multivariate statistical method, canonical correlation analysis or CCA and here we analysed DNA pattern recognition using canonical correlation algorithm.

2. Methodology

2.1 *Genomic sequence dataset*

We have taken *Homo sapiens* beta hemoglobin coding sequences (HBB) for proposed simulation. A hemoglobin molecule contains two alpha hemoglobin and two beta hemoglobin chains. The alpha as well as beta chains is coded by separate genes. The alpha hemoglobin gene is found on chromosome 16, and the beta hemoglobin gene is found on chromosome 11. A sequence of 444 nucleotide bases from beta hemoglobin sequence of the human genome is downloaded from GenBank with accession number NM_000518.4 from 51 to 494.

2.2 *Canonical correlation analysis*

Canonical correlation analysis is to find two sets of basis vectors for two sets of variables which on projections upon their respective basis vectors offer maximal correlation (Al-Kandari and Jolliffe 1997; Kursun *et al.* 2011). The underlying assumption is that the basis vectors X and Y will exist for variables x and y, $\{x(n) \in \mathbb{R}^P, y(n) \in \mathbb{R}^Q; n = 1, 2, \cdots, N\}$ in such a way that the transformed projection upon X and Y are mutually maximized (Hotelling 1936). Thus, canonical correlation analysis finds which directions account for much of the covariance between two data sets.

Canonical correlation analysis computes two projection vectors, $W_x \in \mathbb{R}^P$, $W_y \in \mathbb{R}^Q$ to find the correlation between x and y, such that, the correlation is given as

$$\rho = \frac{E[xy]}{\sqrt{E[x^2]E[y^2]}} = \frac{E\left[W_x^T x y^T W_y\right]}{\sqrt{E\left[W_x^T x x^T W_x\right]E\left[W_y^T y y^T W_y\right]}}$$

$$\rho = \frac{W_x^T C_{xy} W_y}{\sqrt{W_x^T C_{xx} W_x W_y^T C_{yy} W_y}} \quad (1)$$

C_{xy} is the covariance matrix of x and y. C_{xx} and C_{yy} are the dispersion matrices of *x* and *y*, respectively.

The maximum value of ρ with respect to W_x and W_y is the maximum canonical correlation or simply canonical correlation (CC):

$$\rho(x; y) = \max_{W_x \ W_y} \frac{W_x^T C_{xy} W_y}{\sqrt{W_x^T C_{xx} W_x W_y^T C_{yy} W_y}} \quad (2)$$

To maintain the invariance of ρ subject to the scaling of vectors W_x and W_y, CC can be expressed as the following optimization problem:

$$\max_{W_x \ W_y} \ W_x^T C_{xy} W_y$$
$$\text{subject to} \ W_x^T C_{xx} W_x = W_y^T C_{yy} W_y = 1 \quad (3)$$

Assuming C_{yy} as nonsingular, one can obtain W_x by solving the optimization problem

$$\max_{W_x} \ W_x^T C_{xy} C_{yy}^{1} C_{yx} W_x$$
$$\text{subject to} \ W_x^T C_{xx} W_x = 1 \quad (4)$$

The eigenvectors corresponding to top eigenvalues are determined from the following generalized eigenvalue problem:

$$C_{xx}^{1} C_{xy} C_{yy}^{1} C_{yx} W_x = \rho^2 W_x \quad (5)$$

The eigenvalues ρ^2 are the squared canonical correlations. The eigenvectors, W_x and W_y are the normalized canonical correlation basis vectors. The maximum number of canonical correlations are restricted to the minimum dimensionality of x and y. For example, if the dimensionality of x and y is 10 and 6 respectively, the maximum number of canonical correlations is 6.

2.3 *Nucleotide density*

CCA analyzes were done by introducing a *w*-wide window sliding in base-by-base manner along the sequence between position *i* = 1 to 444 region of *Homo sapiens* beta

First-principles calculations of the structural, phonon and thermal properties of ZnX (X = S, Se,Te) chalcogenides

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Abstract

Zinc chalcogenides, ZnX (X = S, Se and Te), are investigated with the full-potential linear-augmented plane wave method within the framework of the density functional theory for their structural, phonon and thermal properties. We consider the generalized gradient approximation for the purpose of exchange-correlation energy determination. Murnaghan's equation of state is used for volume optimization by minimizing the total energy with respect to the unit cell volume. The elastic constants are calculated to examine the crystal structure stability, binding properties and bond character of zinc chalcogenides. By means of frozen-phonon method within the harmonic approximation, we work out phonon dispersion, lattice dynamics and thermal properties of ZnX compounds. The phonon frequencies in the first Brillouin zone, at the zone centre (Γ) and at the zone boundary (X or L) are estimated. The calculated lattice parameters and thermal parameters are in good agreement with other theoretical calculations as well as with the available experimental data.

Keywords: density functional theory, FP-LAPW+l0, Zn-chalcogenides, phonon dispersion, thermal properties

(Some figures may appear in colour only in the online journal)

1. Introduction

During the last decade, a great deal of attention has been devoted to the study of ZnX chalcogenides (X = S, Se, Te) as a member of the broad band gap semiconductor family. They have been shown much interest from a technological point of view and they have gained a reputation for their applications in a variety of opto-electronic devices such as light-emitting diodes, photovoltaic detectors, optical wave guides, modulators and lasers. In particular, zinc selenium, having the distinct property of reversible transformation [1], is utilized in the manufacturing of optical memory devices. These chalcogenides are broadly used for diverse applications in numerous fields such as optical recording due to their excellent sensitivity in laser writing and photography. They have a variety of electrographic applications, such as photoreceptors in photocopying, laser printing, infrared

spectroscopy and fibre-optic techniques [2, 3]. From the perspective of semiconductor device technology, it is essential to get detailed knowledge of the different properties of these materials, especially in the design of ZnX-based optoelectronic devices. In recent times, these compounds have been widely studied experimentally for their structural and optical properties [4–8].

Based on density functional theory (DFT) [9], the electronic, structural, dynamical and optical properties for Zn chalcogenides have been extensively studied [10–15]. DFT with a local density approximation (LDA) [16] of the exchange correlation energy has been used for optical properties calculations. The linear muffin-tin orbital model [11] has determined the electronic structures of ZnX compounds. The empirical pseudopotential method has been exploited for the determination of band structure and of the density of states for the ZnX binary compound [13]. The optical spectra have

Novel biomarker for prostate cancer diagnosis by MRS

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TABLE OF CONTENTS

1. ABSTRACT

Magnetic resonance spectroscopy (MRS) is a prospective tool for characterization of the chemical composition of tissues. *In vivo* MRS can be used for metabolite profiling in the prostate tissue to discriminate non-invasively carcinomas and healthy prostate. In this article different prostate metabolites have been discussed and how to exploit the MRS technique for the estimation of metabolites in prostate tissue quantitatively is elucidated. Choline, citrate, creatine, myo-inositol metabolites can be considered as biomarker for localization of malignancy in the prostate and their ratio can be used for the determination of cancer tissue in the prostate gland.

2. INTRODUCTION

The new 'omics' science like 'genomic', 'proteomics' 'metabolomics' is a promising field of science which can provide valuable information for the detection of cancer. Metabolite profiling is one component of metabolomics, which can be used for the investigation of cancer biology. Many cell regulatory processes are characterized through several low-molecular-weight metabolites (1). Metabolomics can detect changes in the distribution and concentration of a broad range of metabolites in biological systems. The metabolite concentration is important rather than the rate of chemical reaction. Determination of metabolic concentration, which

Ab-Initio Calculations of Structural, Electronic, and Optical Properties of $Cd_{1-x}Mn_xTe$

Bimal Kumar Sarkar, *Member, IACSIT*

Abstract—**We have reported ab-initio calculations of the electronic, structural and linear optical properties of Cd₁_xMnxTe compounds. Ab-initio calculations are performed in the framework of full potential linearized-augmented plane-wave plus local orbitals (FP-LAPW+l₀) method based on the density functional theory (DFT) within the generalized gradient approximation (GGA). Murnaghan's equation of state (EOS) is used for volume optimization by minimizing the total energy with respect to the unit cell. The linear optical properties such as dielectric function, reflectivity, and refractive index are obtained. In the plots of the imaginary part of the complex dielectric function, the absorption threshold shifts toward higher energy with the increase in Mn contents.**

Index Terms—**Ab initio calculations, density-functional theory, equations of state, optical properties, dielectric function.**

I. INTRODUCTION

A great deal of attention has been attributed to the study of diluted magnetic semiconductor due of their potential applications in a wide spectrum of optoelectronic devices, photovoltaic solar cells, laser screen materials and various luminescence devices, etc. [1]. $Cd_{1-x}Mn_xTe$ is one of them, especially important due to variation of its electronic and optical properties by changing the Cd:Mn doping. In this paper we have reported the ab-initio calculations for the investigation of electronic, structural, and optical properties of $Cd_{1-x}Mn_xTe$ alloys using full potential linearized-augmented plane-wave plus local orbitals (FP-LAPW+l₀) method based on the density functional theory (DFT) within the generalized gradient approximation (GGA) [2].

II. COMPUTATIONAL DETAILS

FP-LAPW+lo method as implemented in the Wien2k code [3] with GGA parameterized by Perdew, Burke and Ernzerhof (PBE) [4] is employed to deal with the exchange and correlation effects. The equilibrium structural parameters are carried out by optimizing total energy with respect to the unit cell volume using Murnaghan's equation of state [5]. The calculations were done with $R_{MT}k_{max} = 7$, to achieve energy eigen value convergence. R_{MT} is the smallest radius of the muffin-tin (MT) spheres and k_{max} is the maximum value of the wave vector. The wave function has been expanded inside the atomic spheres with the maximum value of the

angular momentum l_{max} as 10. The irreducible Brillouin zone (BZ) has been decomposed into a matrix of $10\times10\times10$ Monkhorst–Pack k-points [6]. The iteration procedure is continued with total energy and charge convergence to 0.0001Ry and 0.001e, respectively [7], [8].

III. RESULTS AND DISCUSSIONS

The $Cd_{1-x}Mn_xTe$ has a cubic symmetry with space group F-43M. The total energy is optimized with respect to the unit-cell volume by fitting Murnaghan's equation of state [5]:

$$E_T(V) = \left[\frac{B_0 V}{B_0'} \frac{(V_0/V)^{B_0'}}{B_0'-1} + 1 \right] + E_0 - \frac{V_o B_o}{B_0'-1} \qquad (1)$$

For x = 0, 0.25, 0.5, 0.75, 1, Table I shows the energy minimization occuring for a_0 = 6.617, 6.548, 6.487, 6.422 and 6.371 Å, which agree well with the experimental values [9]-[11].

TABLE I: EEQUILIBRIUM LATTICE CONSTANT A_0 (Å), BULK MODULUS B_0 (GPA) AND ITS PRESSURE DERIVATIVE B_0' OF $Cd_{1-x}Mn_xTe$

x	a_0(Å)		B_0(GPa)		B_0'	
	Present	Others	Present	Others	Presen	Others
0.0	6.617	6.56 [9]	37.02	–	3.58	–
0.25	6.548	6.481[11]	34.92	44.50[11]	4.54	6.40[11]
0.5	6.487	6.354[10]	35.61	47.10[10]	4.64	4.58[10]
0.75	6.422	6.32 [8] 6.39 [11]	37.78	49.94[8]	4.99	7.46[8]
1.0	6.371	6.26 [9]	36.12	–	3.58	–

Hence well-defined structural properties are sufficient for further study of electronic and optical properties. The equilibrium lattice constants are used to calculate the density of states (DOS) and electronic band structures for $Cd_{1-x}Mn_xTe$ (shown in Fig. 1 and Fig. 2). The zero of the energy scale is set at the Fermi level (E_F). The energy band structures are calculated along the directions containing high symmetry points of the first Brillouin zone, namely W→ L→ Γ→ X→ W→K. Each member of $Cd_{1-x}Mn_xTe$ demonstrates the existence of the valence band maximum and conduction band minimum at the same symmetry point. This confirms the direct energy gap between the top of the valence band and the bottom of conduction band at Γ point. These plots provide a qualitative explanation of the atomic and orbital origins of the different band states.

COMPENSATION EFFECT IN THE AMORPHOUS HYDROGENATED SILICON FROM POINT OF VIEW OF THE BARRIER-CLUSTER MODEL

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ABSTRACT

Although hydrogenated amorphous silicon has its important practical application there still is not any generally accepted model explaining all the physical phenomena on-going in this matter. The aim of this paper is to familiarize the reader with a model allowing to explain the empirically observed compensation effect (Meyer-Neldel rule – MNR). This effect reflects the correlation between activation energy and pre-exponential factor in relation to the activation dependence of electrical conductivity of semiconductors, including a-Si:H. The model assumes that the recombination of carriers is conditioned by emission of series of monoenergetic phonons. The number of emitted phonons is dependent on the activation energy of disordered semiconductor, which influences the probability of recombination and thus the concentration of free electrons. Consideration of the relationship between compensation effect and Urbach rule is also presented.

Keywords: *hydrogenated amorphous silicon, compensation effect, Meyer-Neldel rule, pre-exponential factor, hopping MNR*

1. INTRODUCTION

Amorphous silicon, and its more useful alloy form, hydrogenated amorphous silicon (a-Si:H), has been the subject of investigation for over 30 years [1-3]. Research into a-Si began in England [4], but the major development, the demonstration of doping and the subsequent implementation of devices was made in Scotland by Spear and LeComber [4-7].

A-Si:H is a low-cost, efficient material which is used extensively for electronic devices. The advantages of a-Si:H are particularly evident when considering the photovoltaic application. The a-Si:H has a large optical absorption coefficient, the energy gap can be modulated to allow optimum conversion efficiency for sunlight. It can be alloyed with other elements (carbon, germanium) to create multijunction structures with increased energy conversion efficiency for sunlight.

The intrinsic disorder in amorphous silicon (a-Si) creates broken bonds, which negatively impact the electronic properties of materials. The main role of hydrogen in amorphous silicon is the passivation of the Si dangling bonds to restore a proper energy gap and the semiconducting properties, thus enabling extensive application of a-Si:H in the microelectronics and the photovoltaic industry. However, several questions are still unanswered.

The first report of hydrogenated amorphous silicon solar cells in 1976 [8] sparked worldwide interest as a promising economically viable source of renewable energy. The materials used in the a-Si:H based solar cells are in fact silicon hydrogen alloys which typically contain about 5 to 20 % of hydrogen.

Serious problem of solar cells based on a-Si:H is so called Staebler-Wronski effect [9] associated with light induced degradation of the material. Continuous progress has been made over the years not only in improving the initial properties of a-Si:H based materials but also in reducing their light induced degradation.

Hydrogenated amorphous silicon is still the subject of intense research. Dark conductivity in a-Si:H can be described by two main processes. The first is the standard extended states conduction process. The second conduction process is referred to as variable-range hopping (VRH) conduction. Great attention is paid to the system a-Si / C: H, respectively a-C:H.

2. MEYER-NELDEL RULE AND a-Si:H

Semiconductors are usually characterized by the temperature dependence of their electrical conductivity, σ

$$\sigma = \sigma_0 \exp\left(-\frac{W}{kT}\right), \qquad (1)$$

where σ_0 is a constant and W – activation energy [10]. Activation dependence (1) corresponds to the first of these mechanisms. For many classes of materials, especially amorphous hydrogenated silicon, chalcogenide glasses, and organic semi-insulators, experimental evidence suggests that a correlation exists between the activation energies and pre-exponential factors in the following form [11-15]

$$\sigma_0 = \sigma_{00} \exp(bW) \qquad (2a)$$

or

$$\ln \sigma_0 = \ln \sigma_{00} + bW, \qquad (2b)$$

where b and σ_{00} are constant. This relation can be written as

$$\sigma_0 = \sigma_{00} \exp\left(\frac{W}{kT_{MN}}\right), \qquad \sigma_0 = \sigma_{00} \exp\left(\frac{W}{E_{MN}}\right). \qquad (3)$$

Here $b = 1/kT_{MN} = 1/E_{MN}$. The value $E_{MN} = kT_{MN}$ is the MN-energy and T_{MN} the MN-temperature. Equation (2) is often referred to as the compensation rule, or Meyer-

ORIGINAL PAPER

Mapping the Structural Topology of IRS Family Cascades Through Computational Biology

**Chiranjib Chakraborty · C. George Priya Doss ·
Sanghamitra Bandyopadhyay · Bimal Kumar Sarkar ·
S. A. Syed Haneef**

Abstract Structural topologies of proteins play significant roles in analyzing their biological functions. Converting the amino acid data in a protein sequence into structural information to outline the function of a protein is a major challenge in post-genome research which can add an extra room in understanding the protein sequence–structure–function relationships. In this study, we performed a comprehensive bioinformatics analysis of structural topology of the IRS family members such as IRS-1, IRS-2, IRS-3, IRS-4, IRS-5 and IRS-6. Based on this assessment, we found that IRS-2 encloses the highest number of α helices, β sheets and β turns in the secondary structure topology compared to IRS-1 and IRS-6. IRS family members are rich in serine or leucine residues.

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Among the IRS family members, the highest percentage of serine and leucine was observed in IRS-1 (15 %) and IRS-5 (10 %), respectively. Notably, the highest number of disulphide bonds was observed in IRS-1 (10) which is responsible for structural stability of the protein. Hydrogen bond pattern in α helices and β sheet was recorded in IRS-1, IRS-2 and IRS-6. By conservation analysis, the longest protein IRS-3 was found to be highly conserved among the IRS family members. The cluster of sequence logo present in the N terminus of these cascades was noted, and highly conserved residues in N-terminal region help in the formation of the two highly conserved domains such as PH domain and PTB domain. Results generated from this analysis will be more beneficial to researchers in understanding more about insulin signalling mechanism(s) as well as insulin resistance pathway. We discuss here that bioinformatics tools utilized in this study can play a vital role in addressing the complexity of structural topology to understand structure–function relationships in insulin signalling cascades.

Introduction

Diabetes is an epidemic disorder, which is rapidly growing throughout the world. Currently, it is an alarming situation throughout the globe [1]. Last decade has witnessed the drastic increase in morbidity and mortality of type-1 and type-2 diabetes by affecting the early and middle age group people [2]. More than 90 % of all diabetes cases have been associated with type-2 diabetes [3]. The cause of diabetes varies from case to

INFORMATION PROCESSING IN NETWORK ARCHITECTURE OF GENOME CONTROLLED SIGNAL TRANSDUCTION CIRCUIT. A PROPOSED THEORETICAL EXPLANATION

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CONTENTS: 1. Introduction. 2. Testing the theoretical model. 3. Shannon information theory and the genome controlled signal transduction circuit. 4. Conclusion. 5. Appendix.

KEYWORDS: Shannon information theory, network architecture, genome controlled signal transduction circuit.

ABSTRACT: *In this paper, Shannon information theory has been applied to elaborate cell signaling. It is proposed that in the cellular network architecture, four components viz. source (DNA), transmitter (mRNA), receiver (protein) and destination (another protein) are involved. The message transmits from source (DNA) to transmitter (mRNA) and then passes through a noisy channel reaching finally the receiver (protein). The protein synthesis process is here considered as the noisy channel. Ultimately, signal is transmitted from receiver to destination (another protein). The genome network architecture elements were compared with genetic alphabet $L = \{A, C, G, T\}$ with a biophysical model based on the popular Shannon information theory. This study found the channel capacity as maximum for zero error ($\sigma = 0$) and at this condition, transition matrix becomes a unit matrix with rank 4. The transition matrix will be erroneous and finally at $\sigma = 1$ channel capacity will be localized maxima with a value of 0.415 due to the increased value at σ. On the other hand, minima exists at $\sigma = 0.75$, where all transition probabilities become 0.25 and uncertainty will be maximum resulting in channel capacity with the minima value of zero.*

1. INTRODUCTION

CELLULAR signaling network appears to be the most complex molecular network within cell [1]. Several signal network architectures in metabolic process

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Ceramic Product Development and Commercialization

Support Vector Machine and Relevance Vector Machine for Prediction of Alumina and Pore Volume Fraction in Bioceramics

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The determination of wt% alumina (wa) and pore volume fraction (pv) in alumina-based bioceramics is important in ceramic engineering. This article adopts support vector machine (SVM) and relevance vector machine (RVM) for prediction of wa and pv based on SiC. SVM is firmly based on theory of statistical learning. RVM is based on a Bayesian formulation of a linear model with an appropriate prior that results in a sparse representation. The developed SVM and RVM give equations for prediction of wa and pv. This article gives robust models based on SVM and RVM for prediction of wa and pv.

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Dielectric constants of zinc-blende semiconductors

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Abstract

Empirical formulae are presented relating the dielectric constants of zinc-blende semiconductors with the average atomic number of the constituent atoms. The high-frequency ε_∞ and static ε_0 dielectric constants can be represented by an empirical linear relation that is a simple function of the average atomic number and the product of ionic charges ($Z_a Z_c$). The calculated results are compared with the available experimental data and previous calculations based on phenomenological models.

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1. Introduction

$A^N B^{8-N}$ have been extensively studied because of their technical and scientific importance and because they have zinc-blende crystallographic structure [1–3]. The dielectric constant of a material is one of the key parameters for device design in nearly all fields of modern electronics. Furthermore, it is of fundamental importance for the behavior of charge carriers, dopants, defects and impurities in insulators and semiconductors [4–7]. Recent developments in modeling, through the use of density functional theory (DFT) and increased computational power, have rendered predictions on mechanical properties *ab initio* from theoretical principles relatively straightforward. Hence, calculations of the optical properties of binary and ternary compound semiconductors and semiconductor alloys are now a common sight. Experimental data to verify these predictions are sparse, especially for nonequilibrium systems, and it can be difficult to interpret the accuracy of the published data.

Due to the difficulties associated with experimental processes and their cost, as well as difficulties in obtaining accurate values of physical properties, researchers moved to calculating the physical properties of solids through theoretical methods. But due to the lengthy process and the complicated computational methods involving a series of approximations, such a method has always been complicated [8]. Over the last few years, a number of theoretical calculations based on empirical relations have

become an essential part of material research. In many cases, empirical relations do not give highly accurate results for each specific material, but they can still be very useful. In particular, the simplicity of empirical relations allows a broader class of researchers to calculate useful properties, and often trends become more evident. Empirical concepts such as valence, empirical radii, ionicity and plasmon energy are then useful [9–13]. These concepts are directly associated with the character of the chemical bond and thus provide a means of explaining and classifying many basic properties of molecules and solids.

Recently, Verma and co-workers evaluated the structural, electronic, mechanical and ground state properties of binary and ternary crystals with the help of ionic charge theory [13–16]. This is due to the fact that the ionic charge depends on the number of valence electrons, which changes when a metal forms a compound. Therefore we thought that it would be of interest to give an alternative explanation for dielectric constants of zinc-blende ($A^{II}B^{VI}$ and $A^{III}B^{V}$) semiconductors.

2. Theory

At optical frequencies, let the field acting on any ion of a crystal be expressed as

$$E_{\text{eff}} = E + LP, \tag{1}$$
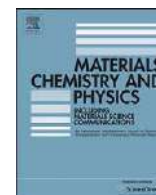
Elastic properties of chalcopyrite structured solids

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ABSTRACT

Elastic properties (i.e. six independent elastic stiffness constants, C_{11}, C_{12}, C_{13}, C_{33}, C_{44} and C_{66}) of chalcopyrite structured solids were evaluated. Values of C_{11}, C_{33}, C_{44}, C_{66}, of $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors exhibit a linear relationship when plotted against the $k_B T_m/\Omega$ (k_B = Boltzmann's constant, T_m = melting temperature, Ω = atomic volume) normalization, but fall on two straight lines according to the product of ionic charges of the compounds. The calculated results are compared with available experimental data and previous calculations based on phenomenological models.

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1. Introduction

Chalcogenide and pnictide semiconductors with the formula $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ have been widely studied because of their possible technological applications as photo-voltaic detectors, solar cells, light emitting diodes, modulators, filters and their use in nonlinear optics [1–5]. These semi-conductors crystallize in the chalcopyrite structure, which is deduced from that of zinc blende by the replacement of the cationic sublattice by two different atomic species. This induces the doubling of the zinc blende unit cell and introduces a tetragonal distortion characterized [6] by the parameter $\eta = c/2a$, where a and c are the lattice parameters, and by the anion displacement $u = 0.25 + (d_{A-C}^2 + d_{B-C}^2)/a^2$ from its position in the cubic cell, where d_{A-C} and d_{B-C} are the cation–anion distances. Because of the added structural (η; u) and chemical ($d_{A-C} \neq d_{B-C}$) degrees of freedom relative to their binary analogue, the ternary semi-conductors exhibit a wide range of interesting physical and chemical properties [2–4]. Although different methods of material preparation for these chalcopyrite ($A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$) compounds have been suggested [6], the knowledge of many of the physico-chemical properties that are essential for designing appropriate conditions for the growth of bulk single crystals and of high-quality epitaxial layers is still inadequate. The elastic properties of these compounds are characterized by six

independent elastic stiffness constants C_{ij}: C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, and C_{66} [7], because of this anisotropy of the elastic properties of these compounds it is evident that the availability of sufficiently large, single phase, homogeneous and defect-free single crystals is an essential precondition for reliable experimental determinations of the elastic constants independent of the specific method used. Table 1 presents the six deformation adapted to the tetragonal $I\bar{4}2d(D_{2d}^{12})$ space group (Laue class $\bar{4}2m$), that we have used to calculate the six elastic constants of chalcopyrite crystals. In general, the strain deformations reduce the symmetry of the cell, eventually increasing the number of degrees of freedom that have to be minimized. Deformations 4–6 in Table 1, for instance, have four internal coordinates of the atoms within the unit cell that are not fixed by symmetry and must be optimized for each deformed cell geometry.

Elastic constants of most of the chalcopyrite family of semi-conductors have not been determined experimentally because of various difficulties in growing single crystals of these compounds [3,8]. Experimental determinations of elastic stiffness constants, compressibilities and bulk moduli for chalcopyrite compounds have been reported in the literature but the results are often contradictory [9]. Attempts have been made to fill this gap in the knowledge of the elastic properties of the chalcopyrites by theoretical calculations using different approaches, but mostly the results obtained differ considerably, and in many cases no satisfactory agreement has been achieved with existing experimental data. On the other hand, the availability of reliable elastic constant data is an essential prerequisite for any calculation or analysis of the influence of pressure, stress and strain on the properties of crystals and thin epitaxial layers.

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Temperature induced band gap shrinkage in Cu$_2$GeSe$_3$: Role of electron–phonon interaction

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A B S T R A C T

The ternary semiconducting compound Cu$_2$GeSe$_3$ has been investigated for optical properties with photoacoustic spectroscopy. Optical absorption spectra of Cu$_2$GeSe$_3$ is obtained in the range of 0.76–0.81 eV photon-energy at temperatures between 80 and 300 K. The thermal variation of band gap energy has been examined from the optical absorption spectra at different temperatures. The temperature induced band gap shrinkage has been explained on the basis of electron–phonon interaction. Varshni's empirical relation in conjunction with Vina and Passler model is taken into consideration for data fitting. The Debye temperature was calculated approximately as 240 K. The acoustic phonons with a characteristic temperature as 160 K corresponding to effective mean frequency have been attributed to the thermal variation of the energy gap.

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1. Introduction

The compound Cu$_2$GeSe$_3$ of low melting point with a small band gap has been investigated for acousto-optic (AO) applications in the IR region [1,2]. It is of the type A$_2^I$B^{IV}C$_3^{VI}$ ternary compounds possessing considerable interest [2–6] as small band gap semiconductors for electro-optic device application. Potential AO materials are selected based on proper choice of low band gaps, low melting points, high atomic weights and high refractive indices. Cu$_2$GeSe$_3$ has a low melting point ($\sim$770 °C) [7] and high refractive index ($\sim$3.2) [8] which enable this material to be used as potential candidate for AO applications in the IR region.

Several researchers have reported different crystal structure of Cu$_2$GeSe$_3$. Earlier Palatnik et al. [9] described its structure as cubic with lattice parameter $a=5.55$ Å. Rivet [10] and Hanh [11] specified Cu$_2$GeSe$_3$ as tetragonal chalcopyrite with unit cell parameters $a=5.595, c=5.482$ Å and $a=5.590, c=10.197$ Å, respectively. Later, on the basis of single crystal analysis, Cu$_2$GeSe$_3$ structure has been reported as orthorhombic with $a=11.860$, $b=3.960$, and $c=5.455$ Å [12]. Further in an X-ray powder diffraction study the same structure was confirmed with the values of a, b and c as 11.878, 3.941, and 5.485 Å, respectively [13]. Thermal and elastic

properties of Cu$_2$GeSe$_3$ were also investigated [14]. Debye's temperature, Young's modulus, specific heat, etc. were obtained from the measurement of thermal expansion, microhardness and velocity of ultrasonic waves. Regarding the applicability of A$_2^I$B^{IV}C$_3^{VI}$ ternary compound as AO material, it is more important to give much emphasis on the investigation of optical properties. From optical absorption measurements [13] the temperature variation of the band gap E_g of Cu$_2$GeSe$_3$ showed band-to-band direct transition with E_g around 0.78 eV at room temperature.

In this paper we present the photoacoustic spectroscopic investigation of optical absorption of Cu$_2$GeSe$_3$ at temperatures T between 70 and 300 K. The temperature dependence of band gap E_g of Cu$_2$GeSe$_3$ has been determined from the photoacoustic signal spectra taken at different temperatures. The theoretical background behind temperature induced band gap shrinkage (BGS) is still controversial. The change of band gap as a function of the temperature results from two contributions: (i) thermal expansion causing change in the band gap energy [15] and (ii) the renormalization of the electronic energies due to electron–phonon interaction [16]. The first contribution is smaller than second one [15,16]. In our work the band gap shrinkage has been explained based on electron–phonon interaction [17]. The temperature dependence of E_g has been generally described by the empirical equation proposed by Varshni [18]. In this work the analytical approaches based on electron–phonon interaction, proposed by Viña et al. [19] and Pässler [20] are taken into consideration to explain the band gap shrinkage and to analyze E_g versus T data for Cu$_2$GeSe$_3$.

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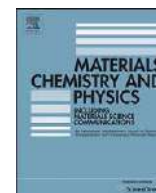
Models for lattice thermal expansion and thermal conductivity for ternary ($A^N B^{2+N} C_2^{7-N}$) tetrahedral semiconductors

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ARTICLE INFO

ABSTRACT

In this paper we have presented two expressions relating the lattice thermal expansion coefficient (α_L, $10^{-6}\,K^{-1}$) and lattice thermal conductivity (K in m W (cm K)$^{-1}$) for $A^{II}B^{IV}C_2^V$ and $A^I B^{III}C_2^{VI}$ semiconductor compounds with the product of ionic charge ($Z_A Z_B Z_C$), melting temperature (T_m) and nearest neighbour distance (d in Å). The lattice thermal expansion coefficient and lattice thermal conductivity of these solids exhibits a linear relationship when plotted on a log–log scale against the melting temperature, but fall on different straight lines according to the product of ionic charge of the compounds. We have applied the modified relations on these solids and found a better agreement with experimental data as compared to the values evaluated by previous researchers so far. The results for lattice thermal expansion coefficient differ from experimental values by an amount up to 5.4% for CdSiP$_2$ and for lattice thermal conductivity the values differ form experiment by an amount up to 3.2% for AgInTe$_2$.

1. Introduction

Thermal properties of the materials are crucial in many industrial applications. Ternary tetrahedral semiconductors have attracted a lot of attention recently [1–6], since they are promising materials for modern microelectronic industries. The ternary compounds are direct gap semiconductors with tetragonal chalcopyrite crystal structure. The chalcopyrite structure is common to compounds of chemical formula $A^{II}B^{IV}C_2^V$ and $A^I B^{III}C_2^{VI}$. The body-centered tetragonal chalcopyrite structure can be derived from the cubic zinc-blende structure by populating one of the face centered cubic sublattices with group B atoms and other one with equal number of group A and C atoms in a regular fashion. Since, generally, A–C and B–C bond lengths, denoted by d_{A-C} and d_{B-C}, respectively, are not equal, the mentioned substitution results in two different structural deformations: the first one is the relocation of anions in the *x*–*y* plane, which is characterized by the parameter $u = 0.25 + (d_{A-C}^2 - d_{B-C}^2)/a^2$. Here, *a* is the lattice constant in the *x* or *y* direction. The second consequence of differing anion–cation bond lengths is a deformation of the unit cell to a length *c* which is equal or smaller than 2*a*. This tetragonal distortion is character-

ized by the quantity $\eta = c/a$ [7]. The importance of these crystals has been well established [1–5], because of their useful design parameters like nonlinear coefficient, appropriate energy band-gap and birefringence. It is the last property which makes the chalcopyrites especially attractive for the various nonlinear laser devices [2,3], i.e. second harmonic generation, sum mixing, difference frequency generation and parametric oscillation covering a broad part of the electromagnetic spectrum from ultraviolet to the infrared through the visible region. Compared to their binary analogues these compounds have higher energy gaps and lower melting points, because of which they are considered to be important in crystal growth studies and device applications. Apart from it, the other important technological applications of these materials are in light emitting diodes, infrared detectors, infrared oscillations, etc. [5–10].

Thermal properties such as lattice thermal expansion coefficient (α_L) and lattice thermal conductivity (K) for many of the chalcopyrite family of semiconductors have not been determined experimentally because of various difficulties in growing proper single crystals of these compounds. Attempts have been made to fill this gap in the knowledge of the thermal properties of the chalcopyrites by theoretical calculations using different approaches, but mostly the results obtained differ considerably, and in many cases no satisfactory agreement has been achieved with existing experimental data [11–17]. The empirical relations have become widely recognized as the method of choice for computational solid-state studies. Modern computational methods have made it possible to

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Inherent properties of binary tetrahedral semiconductors

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ARTICLE INFO

ABSTRACT

A new approach utilising the concept of ionic charge theory has been used to explain the inherent properties such as lattice thermal conductivity and bulk modulus of $A^{III}B^V$ and $A^{II}B^{VI}$ semiconductors. The lattice thermal conductivity (K) of these semiconductors exhibit a linear relationship when plotted on a log–log scale against the nearest neighbour distance d (Å), but fall on two straight lines according to the product of the ionic charge of the compounds. On the basis of this result a simple lattice thermal conductivity–bulk modulus relationship is proposed and used to estimate the bulk modulus of these semiconductors. A fairly good agreement has been found between the experimental and calculated values of these parameters for zinc blende structured solids.

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1. Introduction

Most of the physical world around us and a large part of modern technology are based on solid materials. The extensive research devoted to the physics and chemistry of solids during the last quarter of a century has led to great advances in understanding of the properties of solids in general. So it is interesting to study the behaviour and various properties of different solids. In recent years there has been considerable interest in theoretical and experimental studies of $A^N B^{8-N}$ type crystals with zinc blende structure. It is attributed to their high symmetry and simplicity of their ionic bonding [1]. Almost all the $A^{II}B^{VI}$ and $A^{III}B^V$ compounds crystallize either in the zinc blende or wurtzite structures. The common and dominant feature of these structures is the tetrahedral bonding to four atoms of the other elements. In zinc blende these tetrahedral are arranged in a cubic type structure whilst they are in a hexagonal type structure. Indeed, the centres of similar tetrahedral are arranged in a face-centred cubic (fcc) array in the former and a hexagonal closed-packed (hcp) array in the latter [2]. The particular omnitriangulated nature in atomic structure gives these materials unique physical properties. During the last few years, a number of theoretical calculations based on empirical relations have become an essential part of material research. Because ab initio calculations are complex and required significant effort, more empirical calculations [3,4], have been developed to compute properties of zinc blende solids. The empirical relations have become widely recognized as the method of choice for computational solid-state studies. In modern high-speed computer techniques, it allows researchers to investigate many structural and physical properties of materials only by computation or simulation instead of traditional experiments. Empirical concepts such as valence, empirical radii, electronegativity, ionicity and plasmon energy are then useful [5,6]. These concepts are directly associated with the character of the chemical bond and thus provide means for explaining and classifying many basic properties of molecules and solids.

The valence electrons refer to the electrons that take part in chemical bonding. Recently, Verma and co-authors [7–12] have calculated the electronic, mechanical and optical properties of binary and ternary compounds with the help of ionic charge theory of solids. This is due to the fact that the ionic charge depends on the number of valence electrons, which changes when a metal forms a compound. Therefore, we thought it would be of interest to give an alternative explanation for some inherent properties such as lattice thermal conductivity and bulk modulus of zinc blende solids.

2. Theory, results and discussion

Lattice thermal conductivity and bulk modulus need careful investigation as they are correlated with cohesivity, nature of covalency, bond ionicity and electronic behaviour of the constituent element forming the compound [13,14]. Spitzer [15] and Ioffe [16] experimentally estimated the lattice thermal conductivity (K) of binary and ternary crystals. Different theoretical models, based on bond ionicity and melting temperature, have been proposed by several other researchers [13–16]. The bond ionicity theory of solids has been used by Garbato et al [13] for the calculation of K of the tetrahedral semiconductors and lattice

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Thermal and Optical Properties of $Zn_{1-x}Mn_xTe$ Diluted Magnetic Semiconductor Studied by Photoacoustic Spectroscopic Method

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Abstract   Using photoacoustic spectroscopy, the composition-dependent absorption coefficient (α), thermal diffusivity (σ), and optical bandgap (E_g) of $Zn_{1-x}Mn_xTe$ diluted magnetic semiconductor have been measured. For higher Mn compositions, the absorption spectrum of the Zn–Mn–Te system consists of three regions, viz., the high absorption region, the exponential region, and the weak absorption tail. The bandgap follows a nonlinear variation with composition, showing a downward bowing with a minimum around $x = 0.31$ as a consequence of the electro-negativity difference between the substituted atoms. The composition-dependent band-edge effective mass of the carriers does not show the bowing behavior indicating that the momentum matrix is not the same for all the $Zn_{1-x}Mn_xTe$ alloys due to different lattice constants. The absorption spectra show that the transition is allowed and direct.

Keywords   Absorption coefficient · Diluted magnetic semiconductor · Optical bandgap · Photoacoustic spectroscopy · Thermal diffusivity

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Temperature dependence of elastic constants for ionic solids

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ABSTRACT

In this paper the thermal variation of volume for NaCl, KCl, MgO and CaO has been investigated on the basis of Anderson model. We have evaluated the values of elastic constants C_{11}, C_{44} and K_T at different temperature on the basis of Murnaghan and Tallon models. Tallon's model with second approximation presents slightly better agreement with experimental results which shows that the Anderson–Grüneisen parameter is directly proportional to the volume ratio. Tallon's model can be used to evaluate the values of elastic constants for solids at different temperatures.

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1. Introduction

For proper design and selection of solids for their thermal properties it is very important to have the sufficient knowledge about the thermal variation of elastic properties of solids. A lot of investigations have been done to characterize the thermal variations of elastic properties for ionic solids [1–11]. A number of existing equations of states (EoSs) can be reviewed from Anderson's book on equation of states of solids [12]. To make a good understanding for the equation of state for an ionic solid, the analysis of temperature dependence behaviour of elasticity is more informative than the thermal variation of volume. Moreover information regarding volume change can be realized from the compressibility variation. Though theoretical background in the thermoelastic properties is already there [12], still a complete general theory is lacking. Anderson [13] has reported the experimental data for temperature dependence of thermodynamic and elastic properties for many solids. Here we report a theoretical fitting of thermal variations of elastic constants for some ionic rock salt based cubic structured solids of structure AB type. The elastic properties of these solids such as the bulk modulus and the shear moduli are described in terms of independent second-order elastic constants, viz. C_{11}, C_{12} and C_{44}.

The EoSs are of three categories namely, based on finite strain, assumed relationships between the variables, and interatomic potentials [12]. EoS based on finite strain is straightforward in a sense that the strain can be uniquely determined by stress. The models due to Murnaghan [13] and Tallon [14] are EoS based on finite strain. In this paper we have presented a theoretical calculation of the temperature dependence of elastic constants for NaCl, KCl, MgO and CaO based on Murnaghan and Tallon models. The results are compared with the experimental values of elastic constants at deferent temperatures. The Debye temperature (θ_D) for NaCl and KCl are close to room temperature (304 and 230 K), whereas those for CaO and MgO are much higher (945 and 670 K). We have taken a temperature range from room temperature to 950 K for NaCl, KCl and upto 2800 K for CaO and MgO.

2. Method of analysis

For investigating the temperature dependence of isothermal bulk modulus (K_T), Anderson introduced a parameter which is known as the Anderson–Grüneisen parameter and is defined as follows [12,15]:

$$\delta_T = -\frac{1}{\alpha K_T}\left(\frac{\partial K_T}{\partial T}\right)$$

where α is the coefficient of volume thermal expansion, and T is the temperature. δ_T is related to Grüneisen parameter (γ) as

$$\delta_T = \left(\frac{\partial \ln \gamma}{\partial \ln V}\right)_T + K_T' - 1 \qquad (1)$$

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A R T I C L E

Variations of Water Uptake, Lipid Consumption, and Dynamics during the Germination of *Sesamum indicum* Seed: A Nuclear Magnetic Resonance Spectroscopic Investigation

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Germination in sesame seeds (*Sesamum indicum* L.) in water and in indole-3-acetic acid (IAA) solution is investigated with magic-angle-spinning (MAS) solid state nuclear magnetic resonance (NMR) spectroscopy, supplemented by liquid state NMR spectroscopy. The spectra show good resolution and can be assigned with sufficient confidence. The characteristic spectral peaks and relaxation rates were monitored during the entire course of germination for better understanding of the biophysical and biochemical mechanisms involved in the triphasic water uptake of the seed. A highly positive correlation is found between water uptake and lipid consumption during germination. No significant variation is observed in the relaxation times for the lipid protons during the first two stages of triphasic water uptake, while evident differences are observed for water proton relaxation rates in all stages. Although the total amount of water uptake is largely not changed as a result of IAA, the addition of IAA in seed-germination medium has shown some prominent effects on the germination process, e.g, it suppresses lipid consumption and water mobility, and it reduces the longitudinal and transverse relaxation times of lipid protons and causes a more scattered range for these parameters.

INTRODUCTION

Dormancy is the general characteristic of all seeds, the degree of which defines what conditions should be satisfied to make the seed germinate (*1*). It also occurs for the seed whose embryo is immature and, in some cases, largely undifferentiated such that further development is needed (*2*). Irrespective of embryo maturity, seeds may be called dormant in the sense that germination is blocked physiologically. Several hypotheses have been proposed to explain the mechanisms of dormancy and the modes of action of dormancy-relieving treatments (*3−5*). Under favorable conditions, the quiescent dry seed goes to the nondormant state and germinates as a manifestation of radicle protrusion, i.e., the emergence of the radicle tip through all seed covering layers in association with the elongation of the embryonic axis (*3*). Water uptake plays an important role in the initiation and completion of seed germination. During this process, the dry seed executes triphasic water uptake (*5*), with a quick initial uptake (phase I, i.e., imbibition) followed by a plateau phase (phase II), and a further increase in water uptake (phase III). Also, hormonal changes play a key role in the germination process (*6*). Indole-3-acetic acid (IAA) was proved to be involved in the early stages of

germination in Scots pine seedlings (*7*). Not much investigation of IAA activities on the germination of seed has been done so far, which motivated us to explore the possible effects of IAA on the germination of sesame seeds (*Sesamum indicum* L.).

Identification and quantification of the metabolites of a tissue or an organism is fundamentally important for the study of the biology or physiology of, e.g., plants (*8*). To achieve this objective, it is necessary to make use of a range of analytical methods. Mass spectrometry (MS) is a powerful and rather straightforward tool for such types of analysis and is widely used by chemists and biologists, but complementary information from other techniques, particularly nuclear magnetic resonance (NMR) spectroscopy, is invaluable for the identification of plant metabolites. It is well known that the primary plant metabolites are mainly composed of a few elements including hydrogen, carbon, nitrogen, oxygen, phosphorus, and sulfur. All of these elements with the exception of sulfur have magnetic isotopes that can be detected by NMR. Therefore, NMR signals can be used to identify metabolites in plant tissues and their extracts. Also, it is possible to record a series of in vivo spectra from the same sample and then to interpret the metabolic response of the plant material to any change in its physiological state. Simultaneous acquisition of plant metabolism with in vivo ^{1}H NMR spectroscopy and mass spectrometry was first demonstrated in root tissues (*9*). Some

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