# List of Publications

## Journals

27. Bond length variation in Zn substituted NiO studied from extended X-ray absorption fine structure
S.D. Singh, , A.K. Poswal, **C. Kamal**, P. Rajput, A. Chakrabarti, S.N. Jha, T. Ganguli
*Solid State Communications **259**, 40 (2017)*

26. High-pressure studies on the properties of FeGa3: Role of on-site Coulomb correlation
D. Mondal, V. Srihari , **C. Kamal**, H. Poswal , A. B. Garg, A. Thamizhavel, S. Banik, A. Chakrabarti, T. Ganguli, S. M. Sharma
*Physical Review B, **95**, 134105 (2017)*

25. Structural and magnetic studies on (Fe, Cu) co-doped ZnO nanocrystals
N. Tiwari, , A. Lohar, **C. Kamal**, A. Chakrabarti, C.L. Prajapat, P.K. Mishra, P. Mondal, B. Karnar, N. L. Misra, S. N. Jha, D. Bhattacharyya
*Journal of Physics and Chemistry of Solids **104**, 198 (2017)*

24. Direct Band Gaps in Group IV-VI Monolayer Materials: Binary Counterparts of Phosphorene
**C. Kamal**, A. Chakrabarti, M. Ezawa
*Physical Review B, **93**, 125428 (2016)*

23. Electronic Structure of FeAl Alloy Studied by Resonant Photoemission Spectroscopy and Ab initio Calculations
D. Mondal , S. Banik, **C. Kamal**, M. Nand, S. N. Jha, D. M. Phase, A. K. Sinha, A. Chakrabarti, A. Banerjee, T. Ganguli
*Journal of Alloys and Compounds **688**, 187 (2016)*

22. Structural and electronic properties of $Fe(Al_xGa_{1-x})_3$ system
D. Mondal, **C. Kamal**, S. Banik, A. Bhakar, A. Kak, G. Das, V. R. Reddy, A. Chakrabarti, T. Ganguli
*Journal of Applied Physics **120**, 165102 (2016)*

21. Local structure investigation of (Co, Cu) co-doped ZnO nanocrystals and its correlation with magnetic properties
N. Tiwari, S. Doke, A. Lohar, S. Mahamuni, **C. Kamal**, A.Chakrabarti, R.J. Choudhary, P. Mondal, S.N. Jha, D. Bhattacharyya
*Journal of Physics and Chemistry of Solids, **90**, 100, (2016)*

20. Correlation of size and oxygen bonding at the interface of Si nanocrystal in Si-SiO2 nanocomposite: A Raman mapping study
E. Rani, A. Ingale, A. Chaturvedi, **C. Kamal**, D. M. Phase, M. P. Joshi, A. Chakrabarti, A. Banerjee, L. M. Kukreja
*Journal of Raman Spectroscopy, **47**, 457 (2016)*

19. Aluminene as Highly Hole Doped Graphene
**C. Kamal**, A. Chakrabarti, M. Ezawa
*New Journal of Physics, **17**, 083014 (2015)*

18. Arsenene: Two-dimensional buckled and puckered honeycomb arsenic systems
**C. Kamal** and M. Ezawa
*Physical Review B, **91**, 085423 (2015)*

17. Silicene: A Promising Surface to Achieve Morphology Transformation in Gold Clusters
K. Mondal , **C. Kamal**, A. Banerjee , A. Chakrabarti, T. K. Ghanty
*Journal of Physical Chemistry C, **119**, 3192 (2015)*

16. *Ab initio* Investigation on Hybrid Graphite-like Structure Made up of Silicene and Boron Nitride
**C. Kamal**, A. Chakrabarti, A. Banerjee
*Physics Letters A, **378**, 1162 (2014)*

15. Local Structure Investigation of Co and Mn Doped ZnO Nanocrystals and its Correlation with Magnetic Properties
S. Basu, D. Inamdar, S. Mahamuni, A. Chakrabarti, **C. Kamal**, G. Kumar, S. N. Jha, D. Bhattacharyya
*Journal of Physical Chemistry C, **118**, 9154, (2014)*

14. Experimental and first principle studies on electronic structure of $BaTiO_3$
A. Sagdeo, H. Ghosh, A. Chakrabarti, **C. Kamal**, T. Ganguli, D. M. Phase, S. K. Deb
*AIP Conf. Proc., **1591**, 1142 (2014)*

13. Ab initio Studies of Effect of Intercalation on the Properties of Single Walled Carbon and Gallium Phosphide Nanotubes
**C. Kamal**, A. Chakrabarti, A. Banerjee, S. K. Deb
*Physica E:Low-dimensional Systems and Nanostructures, **54**, 273 (2013)*

12. Silicene Beyond Mono-layers - Different Stacking Congurations And Their Properties
**C. Kamal**, A. Chakrabarti, A. Banerjee, S. K. Deb
*Journal of Physics: Condensed Matter, **25**, 085508 (2013)*

11. How Universal are Hydrogen Bond Correlations ?: A Density Functional Study of Intramolecular Hydrogen Bonding in Low-Energy Conformers of $\alpha$ - amino acids
L. M. Ramaniah , **C. Kamal** , R. J. Kshirsagar , A. Chakrabarti, A. Banerjee
*Molecular Physics, **111**, 3067 (2013)*

10. Density functional investigation on the structures and properties of Li atom doped Au20 cluster
K. Mondal , T. K. Ghanty , A. Banerjee , A. Chakrabarti and **C. Kamal**
*Molecular Physics, **111**, 725 (2013)*

9. First principles DFT study of weak C-HO bonds in crystalline amino acids under pressure-alanine
L. M. Ramaniah, **C. Kamal** and S. K. Sikka
*AIP Conf. Proc., **1512**, 110 (2013)*

8. Nonlinear Optical Properties of Au19M (M = Li, Na, K, Rb, Cs, Cu, Ag) Clusters
A. Banerjee, T. K. Ghanty, A. Chakrabarti, and **C. Kamal**
*Journal of Physical Chemistry C, **116**, 193 (2012)*

7. Interesting Periodic Variations in Physical and Chemical Properties of Homonuclear Diatomic Molecules
**C. Kamal**, A. Banerjee, T. K. Ghanty, and A. Chakrabarti
*International Journal of Quantum Chemistry, **112**, 1097 (2012)*

6. Density Functional Study of α-amino acids : Structural, Energetic and Vibrational Properties
L. M. Ramaniah, A. Chakrabarti, R. J. Kshirsagar, **C. Kamal**, A. Banerjee
*Molecular Physics, **109**, 875 (2011)*

5. The van der Waals coefficients between carbon nanostructures and small molecules: A time-dependent density functional theory study
**C. Kamal**, T. K. Ghanty, A. Banerjee, and A. Chakrabarti
*Journal of Chemical Physics, **131**, 164708 (2009)*

4. Ab initio study of stoichiometric gallium phosphide clusters
**C. Kamal**, T. K. Ghanty, A. Banerjee, and A. Chakrabarti
*Journal of Chemical Physics, **130**, 024308 (2009)*

3. Comparison of electronic and geometric structures of nanotubes with subnanometer diameters: A density functional theory study
**C. Kamal** and A. Chakrabarti
*Physical Review B, **76**, 075113 (2007)*

2. Martensitic transition, ferrimagnetism and Fermi surface nesting in Mn2NiGa
S. R. Barman, S. Banik, A. K. Shukla, **C. Kamal** and A. Chakrabarti
*Europhysics Letters, **80**, 57002 (2007)*

1. Calculation of ground- and excited-state energies of confined helium atom
A. Banerjee, **C. Kamal** and A. Chowdhury
*Physics Letters A, **350**, 121 (2006)*

## Conferences

19. Silicene supported gold clusters: A density functional study
K. Mondal, **C. Kamal**, A. Banerjee, A. Chakrabarti and T.K. Ghanty
*Gordon Research Conferences: Clusters and Nanostructures, Girona, SPAIN (5 - 10 July 2015)*

18. Effect of Al Substitution on the Physical Properties of Intermetallic Semiconductor FeGa3
D. Mondal, **C. Kamal**, S. Banik, Ashok Bhakar, Ajay Kak, G. Das, A.Chakrabarti, and T. Ganguli *International Conference on Condensed Matter and Applied Physics (ICC 2015), Bikaner, Rajastan, INDIA (30 - 31 Oct 2015)*

17. Silicene - a graphene-like structure made up of silicon : A detailed DFT study
**C. Kamal** (Invited talk)
*International Conference "Superstripes 2014", Symposium T: Silicene, the Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Sicily, ITALY (25 - 31 July 2014)*

16. Computational Studies on Two Dimensional Graphene-like Structures
**C. Kamal** (Invited talk)
*Workshop on Advances in Computational Physics (ACP2013), Central University of Tamil Nadu, Thiruvarur, INDIA (14-16 February 2013)*

15. DFT Softwares and Limitations
**C. Kamal** (Invited talk)
*School on Density Functional Theory as a part of National Symposium on Plasma Science and Technology (Plasma-2012), Pondicherry University, Puducherry, INDIA (10 - 12 Dec 2012)*

14. Ab initio Studies On Properties Of Graphene-like Honeycomb Structures
**C. Kamal**, A. Chakrabarti, A. Banerjee and S. K. Deb
*An Advanced School On Modeling Transition Metal Oxides (ATHENA-2012), S. N. Bose National Centre for Basic Sciences, Kolkata, INDIA (09 - 12 Apr, 2012)*

13. Tuning the Properties of Tetrahedral Au20 Cluster by Li Doping K. Mondal, **C. Kamal**, A. Chakrabarti, A. Banerjee, T. K. Ghanty *DAE-BRNS- 4th Interdisciplinary Symposium On Materials Chemistry (ISMC 2012), Bhabha Atomic Research Center, Mumbai (11 - 15 Dec, 2012)*

12. Properties oF Au20 clusters
A. Banerjee, T. K. Ghanty, A. Chakrabarti, K. Mondal, and **C. Kamal**
*DAE-BRNS Symposium on Atomic, Molecular and Optical Physics (2012), Indian Institute of Science Education and Research, Kolkata, INDIA (14 - 17 Dec, 2012)*

11. The van der Waals interaction between diatomic molecules
**C. Kamal**, A. Banerjee, T. K. Ghanty and A. Chakrabarti
*Topical Conference on Interaction of EM Radiation with Atoms, Molecules and Clusters (TC -2010), Raja Ramanna Centre for Advanced Technology, Indore, INDIA (03 - 06 Mar, 2010)*

10. Electronic structures of transition metal doped group IV and III-V nanotubes
A. Chakrabarti and **C. Kamal**
*Psi-K conference 2010, Henry Ford Building, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, GERMANY ( 12 - 16 Sep, 2010)*

9. First Principles Study of Linear and Nonlinear Optical Response Properties of some Amino Acids
A. Chakrabarti, **C. Kamal**, A. Banerjee and L. M. Ramaniah
*DAE-BRNS National Laser Symposium (NLS-19), Raja Ramanna Centre for Advanced Technology, Indore, INDIA (01 - 04 Dec, 2010)*

8. The van der Waals interaction between carbon nanotubes, fullerenes and small molecules
**C. Kamal**, T. K. Ghanty, A. Banerjee, and A. Chakrabarti
*International Conference on Materials for Advanced Technologies (ICMAT 2009), Symposium H: Carbon nanotubes: Synthesis, Characterization and Applications, Suntec Singapore International Convention & Exhibition Centre, SINGAPORE (28 Jun - 03 Jul, 2009)*

7. Structure and Polarizability of Aluminium Phosphide Clusters
   **C. Kamal**, T. K. Ghanty ,A. Banerjee and A. Chakrabarti
   *2nd DAE-BRNS International Symposium on Materials Chemistry (ISMC-2008), Bhabha Atomic Research Center, Mumbai, INDIA ( 02 -06 Dec, 2008)*

6. Electronic and Optical Properties of Amino Acids: A Density Functional Theory Study
   L. M. Ramaniah, A. Chakrabarti, **C. Kamal** and A. Banerjee
   *2nd DAE-BRNS International Symposium on Materials Chemistry (ISMC-2008), Bhabha Atomic Research Center, Mumbai, INDIA ( 02 -06 Dec, 2008)*

5. Time-dependent density functional theory calculation of van der Waals coefficients of small sodium and carbon clusters and C60
   **C. Kamal**, A. Banerjee and A. Chakrabarti
   *52nd DAE Solid State Physics Symposium (DAE-SSPS 2007) , University of Mysore, Mysore, INDIA (27 - 31 Dec, 2007)*

4. Interesting Trends in Electronic structure of ultra-small Carbon nanotubes: A first principles study
   **C. Kamal** and A. Chakrabarti
   *International Conference on Advanced Materials (IUMRS-ICAM 2007), Hotel Grand Ashok, Bangalore, INDIA (08 - 13 Oct, 2007)*

3. Electronic Structure of small carbon and silicon nanotubes
   **C. Kamal** and A. Chakrabarti
   *Eighth International Conference on Optoelectronics, Fiber-optics and Photonics (Photonic-2006), University of Hyderabad, Hyderbad, INDIA (13 - 16 Dec, 2006)*

2. In search of zeta phase in the cation-rich (001) surface of III-V phosphides
   C.Kamal, A. Chakrabarti and A.K.Nath
   *Sixth National Laser Symposium (NLS-2006), Raja Ramanna Centre for Advanced Technology, Indore, INDIA (05 - 08 Dec, 2006)*

1. Electronic Structure of small carbon nanotubes
   **C. Kamal** and A. Chakrabarti
   *International Conference on Laser and Nanomaterials (ICLAN-2006), University of Calcutta, Kolkata, INDIA (30 Nov - 02 Dec, 2006)*

## Chapters in Books

2. Properties of Two-Dimensional Silicon versus Carbon Systems
   **C. Kamal**, A. Banerjee, and A. Chakrabarti
   *Chapter 15, Pages 221-234,Graphene Science Handbook: Size-Dependent Properties, Edited by, M. Aliofkhazraei, N. Ali, W. I. Milne, C. S. Ozkan, S. Mitura, J. L. Gervasoni, CRC Press, Taylor & Francis Group (Invited article)*

1. Properties of Nanomaterials from First Principles Study
   A. Banerjee, A. Chakrabarti, **C. Kamal** and T. K. Ghanty
   *Chapter 20, Pages 527-548, Theoretical and Computational Developments in Modern Density Functional Theory, Edited by Amlan K. Roy, Nova Science Publishers, Inc.*

## RRCAT Report

4. Direct Band Gap in Phosphorene-like Group IV-VI Monolayers
   **C. Kamal**
   *RRCAT Newsletter, 29, 12 (2016)*

3. The van der Waals Coefficients between Carbon Nanostructures and Small Molecules using Time-Dependent Density Functional Theory
   **C. Kamal**, T. K. Chanty, A. Banerjee, A. Chakrabarti
   *RRCAT Newsletter, 23, 18 (2010)*

2. Properties of Nanomaterials from First Principles Study
   A. Chakrabarti, A. Banerjee, **C. Kamal**, T. K. Chanty
   *RRCAT Newsletter, 23, 29 (2010)* (Theme Article)

1. Abinitio study of the electronic and geometric structures of ultra-small single walled nanotubes
   **C. Kamal** and A. Chakrabarti
   *RRCAT Newsletter, 20, 19 (2007)*