CV

Prof. Ajay Chaudhari
Professor and Head
Dept. of Physics
The Institute of Science
Dr. Homi Bhabha State University
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ACADEMIC RECORD

Ph. D. (Physics) : Dr. B. A. M. University, Aurangabad, (M.S.) India **(1997)**

POSITIONS and PROFESSIONAL EXPERIENCE

- June 2019 – till Date — **Professor and Head**, Dept. of Physics
  The Institute of Science,
  Dr. Homi Bhabha State University
  15 Madam Cama Road, Mumbai-400032
- July 1, 2017 – June 2019 — **Professor**, Dept. of Physics
  Govt. Vidarbha Institute of Science and Humanities
  VMV Road, Amravati -444604
- Dec. 27, 2011 – June 30, 2017 — **Professor and Head** Dept. of Physics
  The Institute of Science,
  15 Madam Cama Road, Mumbai-400032
- July 2006 - Dec. 2011 — **Asst. Prof.**, School of Physical Sciences,
  S. R. T. M. University, Nanded – 431 606
- July 2004 – June 2006 — **Postdoctoral Fellow**, Department of Physics, Pennsylvania State University, University Park, Pennsylvania, **USA.**
- Dec. 2000 – May 2004 — **Postdoctoral Fellow**, Department of Chemistry and Biochemistry, National Chung-Cheng University, Ming-Hsiung, ChiaYi, **Taiwan (R.O.C.).**

AWARDS, FELLOWSHIP AND MEMBERSHIP

- Postdoctoral Fellowship by **National Science Council, Taiwan (2000-2004).**
- Postdoctoral fellowship by **Material Research Institute, Pennsylvania State University, University Park, Pennsylvania, USA (2004-2006)**
- Visiting Associate of **Inter University Centre for Astronomy and Astrophysics, Pune (2008-2011)**

- Life member of **Indian Physics Association (IPA)**
- Life member of **Indian Association of Physics Teachers (IAPT)**
- Life member of **Indian Science Congress Association (ISCA)**

RESEARCH INTEREST

- Computational Materials Science
- Nanomaterials for Hydrogen storage, Gas sensing and NLO applications
- Density Functional Theory
- Interstellar molecules
- Hydrogen bonding
- Monte Carlo simulation
- Dielectric relaxation

RESEARCH PROJECTS

Sr. No.	Title of Project	Funding Agency	Tenure
1	Quantum Chemical study of Hydrogen Storage in metal decorated compounds	C.S.I.R.	2013-2016
2	Computational study of hydrogen storage capacity of organometallic compounds using Density Functional Methods	C.S.I.R.	2008-2011
3	Theoretical study of cosmic molecules : A quantum chemical approach	ISRO	2008-2012

CANDIDATES REGISTERED/COMPLETED Ph.D/M.Phil. DEGREE

Sr. No.	Name of candidate	Date of award/Status
1	**Mrs. Gul Afroz Meraj**	**Oct. 9, 2010 (M.Phil)**
2	**Mr. Nitin Wadnerkar**	**Nov.21, 2011 (Ph.D.)**
3	**Mr. Vijayanand Kalamse**	**Feb. 21, 2012 (Ph.D.)**
4	**Mr. Mahadevappa Naganathappa**	**Feb. 27, 2012 (Ph.D.)**
5	**Mr. Vinayak Deshmukh**	**Aug.24, 2012 (Ph.D.)**
6	**Mr. Bhagwat Kharat**	**Aug.24, 2012 (Ph.D.)**
7	**Mrs. Gul Afroz Meraj**	**June 27, 2015 (Ph.D.)**
8	**Ms. Priyanka Tavhare**	**Aug. 20, 2015 (M.Phil)**
9	**Mr. Ranvinder Konda**	**Aug. 20, 2015 (M.Phil)**
10	**Mr. Ranvinder Konda**	**Oct. 29, 2021 (Ph.D.)**
11	**Mr. Nilesh Ingale**	**Jan. 13, 2022 (Ph.D.)**
12	**Ms. Priyanka Tavhare**	**June 16, 2022 (Ph.D.)**
13	**Mr. Chaitanya Baban Gend**	**Registered**
14	**Ms. Poonam Parkar**	**Registered**
15	**Ms. Unnati Jethawa**	**Registered**

BOOKS/Chapters in Books PUBLISHED

Sr. No	Title	Author's Name	Publisher	Year of Publication
1	Binary Polar Liquids : Structural and Dynamic Characterization Using Spectroscopic Methods	Suresh Mehrotra, Ashok Kumbharkhane and Ajay Chaudhari	Elsevier	2017
2	Organometallic Nanostructures: Hydrogen Storage,Structure, Stability and Kinetics- In- *Advances in Chemistry Research* Vol. 23, (Chapter 6, pp 157-205)	Nitin Wadnerkar, Vijayanand Kalamse and Ajay Chaudhari Editor- James C. Taylor	Nova Science Publishers, Inc. New York, USA	2015
3	Extracting information about surface heterogeneity effect on heterogeneous reactions using multifractal scaling analysis- In- *Heterogeneous Catalysis Research Progress* (Chapter 10 -pp 369-393)	Ajay Chaudhari and Shyi-Long Lee Editor - Mathias B. Gunther	Nova Science Publishers, Inc. New York, USA	2008

PUBLICATIONS

1. M. Mohammadi, H.Y. Abdullah, V. Kalamse, and **Ajay Chaudhari**
   Bromochlorodifluoromethane interaction with pristine and doped BN nanosheets: A DFT study
   J. Env. Chemical Engn. 10, 108367 (2022)
2. Nilesh Ingale, Priyanka Tavharre and **Ajay Chaudhari**
   Hazardous molecules and VOCs sensing properties of Ti functionalized benzene: an ab initio study
   Sensors and Actuators : A. Physical 342, 113657 (2022)
3. Priyanka Tavharre and **Ajay Chaudhari**
   Ti decorated heterocyclic rings for hydrogen storage
   Int. J. Hydrogen Energy 47, 3948-3960 (2022)
4. M. Mohammadi, H.Y. Abdullah, V. Kalamse, and **Ajay Chaudhari**
   Interaction of Halomethane CH_3Z (Z = F, Cl, Br) with $X_{12}Y_{12}$ (X = B, Al, Ga & Y = N, P, As) Nanocages
   Comput. and Theo.Chem. 1208, 113544 (2022)
5. B. Kharat, M. Naganathappa, V. Jagrut and **Ajay Chaudhari**
   Spectroscopy and second hyperpolarizability of singlet, triplet and quintet spin states of acetonitrile
   Spectrochimica Acta, 265, 120389 (2022)
6. M. Mohammadi, H.Y. Abdullah, V. Kalamse, and **Ajay Chaudhari**
   Interaction of Fluorouracil drug with boron nitride nanotube, Al doped boron nitride nanotube and BC2N nanotube
   Comput. and Theo.Chem. 1212, 113699 (2022)
7. S. Kaluva, K. V. Laxmi, **Ajay Chaudhari** and M. Naganathappa

Effect of new DFT methods on spectroscopy and NLO analysis of 2-Bromo-5-nitrothiozole and Nitrosodimethylamine
J. Mol. Mod. 28, 135 (2022)

8. Priyanka Tavhare, Elby Titus and **Ajay Chaudhari**
Hydrogen Adsorption on Metal Functionalized Benzene and B-substituted Benzene
Int. J. Energy Res. 45, 18810-18826 (2021)
9. R. Rahimi, M. Solimannejad, and **Ajay Chaudhari**
Toxic volatile organic compounds sensing by Al_2C monolayer: A first-principles outlook
J. Hazardous Materials, 403, 123600 (2021)
10. R. Rahimi, M. Solimannejad, and **Ajay Chaudhari**
Pristine B_3CN_4 monolayer for hydrogen storage: A first-principles approach
Phys. Letts. A, 391, 127116 (2021)
11. R. Konda, Elby Titus and **Ajay Chaudhari**
Functionalized Boranes and Carboranes for Hydrogen storage: A comparison
Int. J. Energy Res. 45, 7605-7616 (2021)
12. M. Mohammadi, H.Y. Abdullah, V. Kalamse, and Ajay Chaudhari
Adsorption of alkali and alkaline earth ions on nanocages using density functional theory
Comput. And Theo. Chem. 1204, 113391 (2021)
13. M. Naganathappa, B. Kharat, S. Ramesh and **Ajay Chaudhari**
Hydrogen bonded cluster of nitroxyl: Many body analysis and spectroscopic characterization
Struct. Chem. 32, 1163–1170 (2021)
14. R. Konda, M. Solimannejad, and **Ajay Chaudhari**
H_2 storage and Equilibrium Isotope Effect for Be, Li and Ti doped closoborate complexes
Struct. Chem. 32, **1489–1504 (2021)**
15. Nilesh Ingale, Priyanka Tavhare, M. Solimannejad and **Ajay Chaudhari**
Titanium doped benzene as a molecular oxide sensor: A first principles approach
J. Mol. Modeling, 27, 242 (2021)
16. R. Konda, Amol Deshmukh, V. Kalamse and **Ajay Chaudhari**
Functionalized Tetrahedral Silsesquioxane Cages for Hydrogen Storage
Int. J. Hydrogen Energy, 45, 32157-32167 (2020)
17. N. Mahadevappa, B. Kolli, S. Ravula, **Ajay Chaudhari**
NLO properties and spectroscopic characterization of Y-shaped polymer using quantum chemical approach
J. Mol. Modeling, 26, 299 (2020)
18. M. Solimannejad, R. Konda, R. Rahimi, and **Ajay Chaudhari**
Ab initio calculations and molecular dynamics simulation of H_2 adsorption on $CN_3Be_3^+$ cluster
Struct. Chem. 31, 1757-1763 (2020)
19. Nilesh Ingale, R. Konda and **Ajay Chaudhari**
Volatile organic compounds sensing by Li/Ti doped ethylene complex
Adsorption. 26. 103-115 (2020)
20. Priyanka Tavhare and **Ajay Chaudhari**

Ti-doped B/N substituted benzene complexes for hydrogen storage : A Comparison
Materials Letters. 244, 104-107 (2019)

21. Priyanka Tavhare, Elby Titus and **Ajay Chaudhari**
Boron substitution effect on adsorption of H_2 molecules on organometallic complexes
Int. J. Hydrogen energy, 44, 345-353 (2019)
22. Priyanka Tavhare and **Ajay Chaudhari**
Nitrogen substitution effect on hydrogen adsorption properties Ti decorated benzene
Struct. Chem. 30:2151–2158 (2019)
23. M. Naganathappa and **Ajay Chaudhari**
Theoretical and experimental study of dimethyl sulfoxide and N-substituted DMSO
Ind. J. Pure and Appl. Phys. 57, 261-267 (2019)
24. Nilesh Ingale, R. Konda and **Ajay Chaudhari**
Metal doped ethylene complexes for hazardous gas molecule sensing
Struct. Chem. 30, 1057-1066 (2019)
25. R. Konda, Elby Titus and **Ajay Chaudhari**
Adsorption of molecular hydrogen on inorganometallic complexes B_2H_4M (M=Li, Be, Sc, Ti, V)
Struct. Chem. 29, 1593-1599 (2018)
26. Nilesh Ingale, R. Konda and **Ajay Chaudhari**
Gas sensing properties of organotitanium complex from first principles calculations and molecular dynamics simulations
Chem. Phys. Lett. 706, 247-254 (2018)
27. Nilesh Ingale, R. Konda and **Ajay Chaudhari**
Organolithium complex as a gas sensing material for oxides from ab initio calculations and molecular dynamics simulations
Int. J. Quantum Chem. 118, e25623 (2018)
28. Priyanka Tavhare and **Ajay Chaudhari**
Spectroscopic characterization of metal decorated benzene and boron/nitrogen substituted benzene
Ind. J. Pure & Appl. Phys. 56, 341-345 (2018)
29. R. Konda, Priyanka Tavhare, Nilesh Ingale and **Ajay Chaudhari**
Tetrahedral Silsesquioxane-C_2H_2Ti complex for hydrogen storage.
AIP Conference Proceedings, 1942, 140011 (2018)
30. Nilesh Ingale and **Ajay Chaudhari**
Spectroscopic analysis of Sulphur dioxide adsorbed C_2H_4Ti complex: A First Principles study
Ind. J. Pure & Appl. Phys. 56, 331-334 (2018)
31. M. Naganathappa and **Ajay Chaudhari**
Spectroscopic characterization of glycols from density functional theory and experiment.
Vib. Spectroscopy, 95, 7-15 (2018)
32. R. Konda and **Ajay Chaudhari**
Vibrational spectra for closoborate and metal doped closoborate using ab initio method

Ind. J. Pure & Appl. Phys. 56, 265-268 (2018)

33. R. Konda, Amol Deshmukh, Elby Titus and **Ajay Chaudhari**
Alkali, alkaline earth and transition metal doped B_6H_6 complexes for hydrogen storage
Int. J. Hydrogen Energy 42, 23723-23730 (2017)
34. V. Kalamse, Priyanka Tavhare, R. Krishna, E. Titus and **Ajay Chaudhari**
Effect of boron substitution on hydrogen storage capacity of metal decorated napthalene
Int. J. Hydrogen Energy 42, 23716-23722 (2017)
35. Priyanka Tavhare, Amol Deshmukh and **Ajay Chaudhari**
Impact of position and number of boron atom substitution on hydrogen uptake capacity of Li decorated pentalene
Phys. Chem. Chem. Phys. 19, 681-694 (2017)
36. Amol Deshmukh, R. Konda, Elby Titus and **Ajay Chaudhari**
Electronic structure calculations and molecular dynamics simulations of hydrogen adsorption on Beryllium doped complexes
Int. J. Hydrogen Energy 42, 23708-23715 (2017)
37. Amol Deshmukh, R. Konda, V. Kalamse and **Ajay Chaudhari**
Improved hydrogen uptake capacity of transition metal doped benzene by boron substitution
RSC Advances, 6, 47033-47042 (2016)
38. P.Tavhare, Vijayanand Kalamse, R. Krishna, E. Titus and **Ajay Chaudhari**
Hydrogen adsorption on Ce-ethylene complex using quantum chemical methods
Int. J. Hydrogen energy, 41, 11730-11735 (2016)
39. Vijayanand Kalamse, R. Krishna, E. Titus and **Ajay Chaudhari**
Boron substituted and un-substituted aromatic complexes as hydrogen storage media
Int. J. Hydrogen energy, 41, 11723-11729 (2016)
40. P. Tavhare, N. Wadnerkar, V. Kalamse and **Ajay Chaudhari**
H_2 interaction with C_2H_2TM(TM=Sc, Ti, V) complex using quantum chemical methods
Acta Physica Polonica A, 129, 1257-1262 (2016)
41. Vinayak Deshmukh, Bhagawat Kharat and **Ajay Chaudhari**
Hyperpolarizabilities of 1,3,5-triamino-2,4,6-trinitrobenzene using ab initio and Density Functional theory method
Quantum Matter, 5, 492-499 (2016) (ISSN: 2164-7615(print); EISSN:2164-7623 (online)**)**
42. R. Konda, V. Kalamse, Amol Deshmukh and **Ajay Chaudhari**
Closoborates-transition metal complexes for hydrogen storage
RSC Advances, 5, 99207-99216 (2015)
43. M. Naganathappa, T. Qureshi and **Ajay Chaudhari**
Mono and di-substituted ammonia borane : A Computational study
J. Mol. Liquids, 211, 776-783 (2015)
44. M. Naganathappa and **Ajay Chaudhari**
Spectroscopic characterization of Cysteine and Methionine using Density Functional Theory method
Astrophys. and Space Sci., 357, 42 (2015)
45. Priyanka Tavhare, Vijayanand Kalamse, Radhika Bhosale and **Ajay Chaudhari**

Interaction of molecular hydrogen with alkali and transition metal doped acetylene complexes
Struc. Chem. 26, 823-829 (2015)

46. GulAfroz Meraj and **Ajay Chaudhari**
Theoretical investigation of hydrogen bonding interaction in $H_3O+(H_2O)_9$ complex
J. Molecular Modeling, 20, 2480 (2014)
47. V. Deshmukh, M. Naganathappa, B. Kharat and **Ajay Chaudhari**
Theoretical Study of Borazine and Substituted Borazines using Density Functional Theory method
J. Mol. Liquids, 193, 13-22 (2014)
48. GulAfroz Meraj and **Ajay Chaudhari**
Hydrogen bonded hydrated hydronium and Zundel ion complexes
J. Mol. Liquids, 190, 1-5 (2014)
49. Bhagwat Kharat, Vinayak Deshmukh and **Ajay Chaudhari**
Hydrogen bond co-operativity effects in cyclic and ladder cyanamide oligomers using Density Functional Theory Method
J. Mol. Liquids, 186, 131-141 (2013)
50. T. Lin, **Ajay Chaudhari** and Shyi-Long Lee
Correlation between substituent constants and hyperpolarizabilities for di-substituted Trans-azobenzenes
Journal of Molecular Modeling 19, 529-538 (2013)
51. Nitin Wadnerkar, Vijayanand Kalamse and **Ajay Chaudhari**
Hydrogen uptake capacity of C_3H_3-X(X=Sc,Ti) organometallic compounds
Struct. Chem.24, 369-374 (2013)
52. C. K. Chang, Vinayak Deshmukh, **Ajay Chaudhari** and S. L. Lee
Nonlinear optical properties of $(H_2CO)n$ (n=1-7) oligomers using Finite Field and Hyperpolarizability Density analysis approach
J. Computational and Theo. Nanosci. 10, 684-696 (2013)
53. Bhagwat Kharat, Vinayak Deshmukh and **Ajay Chaudhari**
Effect of spin multiplicity on structure, second hyperpolarizability and vibrational spectrum of cynamide
J. Computational and Theo. Nanoscience 10, 19-26 (2013)
54. Vijayanand Kalamse, Nitin Wadnerkar, Amol Deshmukh and **Ajay Chaudhari**
Multi-functionalized naphthalene complexes for hydrogen storage
Energy, 49, 469-474 (2013)
55. Bhagwat Kharat, Vinayak Deshmukh and **Ajay Chaudhari**
Computational study of $(CH_3\text{-}C{\equiv}N)_n$ (n=1-5) oligomers using Density Functional Theory method
J. Mol. Liquids 177, 172-181 (2013)
56. V. Deshmukh, M. Naganathappa, B. Kharat and **Ajay Chaudhari**
Computational study of monosubstituted acetonitrile using quantum chemical methods.
Opt. Materials 35, 353-360 (2013)
57. Nitin Wadnerkar, Vijayanand Kalamse and **Ajay Chaudhari**
Can ionization induce an enhancement of hydrogen storage in Ti_2-C_2H_4 complex?
RSC Advances, 2, 8497-8501 (2012)
58. Mahadevappa Naganathappa, and **Ajay Chaudhari**

Infrared and electronic absorption spectra of $C_{16}H_{10}$ isomers, their ions and doubly ions using Quantum Chemical Methods
Mon. Notices of the Royal Astron. Soc. 425, 490-505 (2012)

59. Bhagwat Kharat, Vinayak Deshmukh and **Ajay Chaudhari**
Hydrogen Bonding Interactions in Acetonitrile Oligomers using Density Functional Theory method
Struct. Chem.23, 637-644 (2012)
60. Vijayanand Kalamse, Nitin Wadnerkar and **Ajay Chaudhari**
Hydrogen storage in C_3Ti complex using Quantum chemical methods and molecular dynamics simulations
J. Molecular Modeling, 18, 2423-2431 (2012)
61. Vijayanand Kalamse, Nitin Wadnerkar, Amol Deshmukh and **Ajay Chaudhari**
Interaction of molecular hydrogen with Ni doped ethylene and acetylene complex
Int. J. Hydrogen Energy, 37, 5114-5121 (2012)
62. Bhagawat Kharat, Vinayak Deshmukh and **Ajay Chaudhari**
Cyclic and ladder hydrogen bonded oligomers of Cyanamide: A Density functional theory and Many-body analysis approach
Struct. Chem. 23, 37-45 (2012)
63. Nitin Wadnerkar, Vijayanand Kalamse, Shyi-Long Lee and **Ajay Chaudhari**
Verification of DFT predicted hydrogen storage capacity of VC3H3 complex using Moecular Dynamics simulations
J. Computational Chem. 133, 170-174 (2012)
64. Vinayak Deshmukh, Shyi-Long Lee and **Ajay Chaudhari**
Co-operativity effects in linear formaldehyde oligomers using Density Functional Theory calculations
J. Mol. Modeling 18, 3723-3729 (2012)
65. Gulafroz Meraj, M. Naganathappa and **Ajay Chaudhari**
Energetics during the proton transfer process in Zundel ion-$4H_2O$ complex
Int. J. Quant. Chem. 112, 1439-1448 (2012)
66. Vijayanand Kalamse, Nitin Wadnerkar, Amol Deshmukh and **Ajay Chaudhari**
C_2H_2M (M=Ti,Li) complex : A possible hydrogen storage material
Int. J. Hydrogen energy, 37, 3727-3732 (2012)
67. Vinayak Deshmukh, Bhagawat Kharat and **Ajay Chaudhari**
Nonlinear optical properties and spectroscopic characterization of aniline in singlet, triplet and quintet state using quantum chemical methods
Computational and Theo. Chem. 980, 115-122 (2012)
68. Mahadevappa Naganathappa, and **Ajay Chaudhari**
Quantum chemical study of glycine and its precursor aminoacetonitrile in gas phase and astrophysical ice
Asian J. of Spectroscopy Special Issue, 195-206 (2012)
69. K. P. R. Nair, M. Konwar, M. Naganathappa and **Ajay Chaudhari**
Molecular structure and vibrational frequencies of o-, m-, and p-fluorotoluene from the theory and Experiment
Asian J. Spectroscopy, Special Issue, 187-194 (2012)
70. Vinayak Deshmukh, Bhagwat Kharat and **Ajay Chaudhari**
Borazine in Singlet, triplet and quintet state: Spectroscopic characterization and Nonlinear optical properties using ab initio and Density Functional theory method

J. Computational and Theoretical Nanoscience 9, 1633-1641 (2012)

71. N.Wadnerkar, V. Kalamse, A.B. Philips, B.S. Shivaram and **Ajay Chaudhari**
Vibrational spectra of Ti:$C_2H_4(nH_2)$ and Ti:$C_2H_4(nD_2)$ (n=1-5) complexes and the Equilibrium Isotope Effect : Calculation and Experiment.
Int. J. Hydrogen energy 36, 9727-9732 (2011)
72. M. Naganathappa and **Ajay Chaudhari**
Effect of ionization on vibrational and absorption spectra of ethyl formate : A computational study
J. Phys. Chem. A 115, 4743-4756 (2011)
73. Nitin Wadnerkar, Vijayanand Kalamse and **Ajay Chaudhari**
VC_3H_3 organometallic compound: A possible hydrogen storage material
Int. J. Hydrogen Energy, 36, 664-670 (2011)
74. M. Naganathappa and **Ajay Chaudhari**
Theoretical study of vibrational and absorption spectra of n-butyronitrile and its ions using Møller Plesset method
J. Mol. Modeling 17, 1695-1705 (2011)
75. M. Naganathappa and **Ajay Chaudhari**
Spectroscopic characterization of aminoacetonitrile, its ions and protonated aminoacetonitrile using quantum chemical methods
Int. J. Quant. Chem. 111, 2064-2071 (2011)
76. **Ajay Chaudhari,** M. Naganathappa, M. N. Shinde and A. C. Kumbharkhane
Theoretical investigation of interaction between dioxane and water using hydrogen bonding model and Density functional Method.
Int. J. Quant. Chem. 111, 2972-2979 (2011)
77. M. Naganathappa, Shivaji Waghmare and **Ajay Chaudhari**
Infrared and electronic absorption spectra of formaldehyde in gas phase and astrophysical H_2O ice
Astrophys. and Space Sci. 332, 249-256 (2011)
78. Vijayanand Kalamse, Nitin Wadnerkar and **Ajay Chaudhari**
Theoretical study of third row transition metal monofluorides
Int. J. Quant. Chem. 111, 2014-2020 (2011)
79. Vijayanand Kalamse, Nitin Wadnerkar and **Ajay Chaudhari**
Hydrogen storage in C_2H_4V and $C_2H_4V^+$ organometallic compound
J. Phys. Chem. C 114, 4704-4709 (2010)
80. Nitin Wadnerkar, Vijay Kalamse and **Ajay Chaudhari**
Hydrogen storage capacity of C_2H_4Sc and its ions : A Density Functional Study
J. Computational Chemistry, 31, 1656-1661 (2010)
81. Ajay Chaudhari, Gulafroz Meraj and Shyi-Long Lee
Many body energies during proton transfer mechanism in aqueous system
J. Mol. Modelling 16, 1559-1566 (2010)
82. Nitin Wadnerkar, Vijayanand Kalamse and **Ajay Chaudhari**
Higher hydrogen uptake capacity of $C_2H_4Ti^+$ than C_2H_4Ti : a quantum chemical study
Theo. Chem. Accts. 127, 285-292 (2010)
83. **Ajay Chaudhari** and Shyi-Long Lee
Microhydration of Hydronium ion and Zundel ion: A Many Body analysis approach
J. Theo. & Comput. Chem. 9, 177-187 (2010)

84. Ajay Chaudhari
Hydrogen bonding interaction between 1,4-dioxane and water
Int. J. Quant. Chem. 110, 1092-1099 (2010)

85. M. Naganathappa and **Ajay Chaudhari**
Absorption and vibrational spectra of methylamine and its ions using Quantum Chemical Methods
Adv. Space Research, 45, 521-526 (2010)

86. Vijayanand Kalamse, Nitin Wadnerkar and **Ajay Chaudhari**
Quantum chemical study of dissociation of H_2 on C_3H_3V organometallic compound
Int. J. Quant. Chem. 110, 1947-1952 (2010)

87. Vijayanand Kalamse, Sanjay Gaikwad and **Ajay Chaudhari**
Computational study of 5d transition metal mononitrides and monoborides using Density Functional method.
Bull. of Mat. Sci. 33, 233-238 (2010)

88. Nitin Wadnerkar, Vijayanand Kalamse and **Ajay Chaudhari**
Hydrogen storage in neutral and charged metalized-CnHm (for n=m and n m) compounds
Proc. of 10th International Conference on Nanotechnology (IEEE NANO 2010), Kintext, Seoul, Korea (Aug- 17-20, 2010)

89. Bhagwat Kharat, S. B. Deshmukh and **Ajay Chaudhari**
4d transition metal monoborides, monocarbides, mononitrides, monoxides and monofluorides: A quantum chemical approach.
Int. J. Quant. Chem. 109(5), 1103-1115 (2009)

90. S. V. Shinde, W. N. Jadhav, N. N. Karde, R. H. Tale and **Ajay Chaudhari**
Synthesis and computational study of substituted pyrimido[4,5-d]-pyrimidine-2-(1H)-one ot thiones
Bull. of Cat. Soc. India, Vol. 8 (4), 157-163 (2009)

91. H. C. Chaudhari, **Ajay Chaudhari** and S. C. Mehrotra
Microwave dielectric characterization of aqueous solutions of Tryptophan
J. Kor. Chem. Soc. 52(4), 350-355 (2008)

92. R.Gacche, M. Khsirsagar, S. Kamble, B. Bandgar, N. Dhole**,** and **Ajay Chaudhari**
Antioxidant and Anti-inflammatory related activities of selected synthetic Chalcones : A structure activity relationship studies using Computational tools.
Chem. Phar. Bull., 56(7), 897-901 (2008).

93. **Ajay Chaudhari** and Shyi-Long Lee
Effect of sticking probability on monomer-dimer reaction
Bull. Cat. Soc. India, 7, 90-95 (2008)

94. D. Suryawanshi, **Ajay Chaudhari**, A.Jadhav, M.Lokhande, A.Kumbharkhane and S. Mehrotra
Hydrogen bonding interaction in Diol-water system using Time Domain Technique and Density Functional Method.
Frontiers of Microwaves and Optoelectronics, Proc. of International Conference on Microwaves and Optoelectronics (ICMO-2007), Dec. 17-20, 670-676 (2007)

95. Jorge Sofo, **Ajay Chaudhari** and Greg Barber
Graphane : the first two-dimensional hydrocarbon
Phys. Rev. B, 75, 153401 (2007)

96. **Ajay Chaudhari** and Shyi-Long Lee
Computer simulation of Eley-Rideal reactions over rough surface
J. Chin. Chem. Soc., 54, 1201-1210 (2007)
97. **Ajay Chaudhari** and Shyi-Long Lee
Theoretical study of first row transition metal mononitrides using density functional theory method
Int. J. Quant. Chem. , 107(1) 212-218 (2007)
98. Ching-Cher Sanders Yan, Wan-Ting Chuang, **Ajay Chaudhari** and S.-L. Lee
Lattice model studies of CO oxidation kinetic oscillation over nano-scaled Pt particle: Effect of temperature variation and diffusion
Appl. Surf. Sci., 252(3), 784-792 (2005)
99. Hui-Yin Wu, **Ajay Chaudhari** and Shyi-Long Lee
Theoretical studies on nonlinear optical properties of Formaldehyde oligomers by ab initio and density functional theory methods
J. Comput. Chem. , 26, 1543-1564 (2005)
100. **Ajay Chaudhari** and Shyi-Long Lee
Computational study of glycine-(water)$_3$ complex by Density functional method
Chem. Phys. 310,281-285 (2005)
101. H. C. Chaudhari, **Ajay Chaudhari** and S. C. Mehrotra
Dielectric study of aqueous solutions of alanine and phenylalanine
J. Chin. Chem. Soc. 52(1), 5-10 (2005)
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