# UNIVERSITY OF CALCUTTA

## FACULTY ACADEMIC PROFILE/ CV

1. **Full name of the faculty member** Debasis Mukhopadhyay
2. **Designation**: Professor
3. **Specialisation** : Physical Chemistry
4. **Passport size photograph** :

5. **Contact information** :

B-36, New Garia Housing Development Cooperative Society,
Kolkata 700094, West Bengal.
e-mail : dm.chem.cu@gmail.com Phone Number : 9831351332

6. **Academic qualifications**:

| College/ university from which the degree was obtained | Abbreviation of the degree |
|---|---|
| B.B. College, Burdwan University | B.Sc.(Honours in Chemistry) |
| Burdwan University | M.Sc. (Chemistry) |
| Jadavpur University(Working Place : Indian Assoc. for the Cultivation of Science, Kolkata) | Ph.D.(Science) |

7. **Positions held/ holding:**

| Institution | Period | Designation |
|---|---|---|
| Ramakrishna Mission Vidyamandira ( A undergraduate College, then affiliated to Calcutta University), Belur Math. | April 15, 1992– April 14, 1997 | Lecturer |
| Do | April 15, 1997 – April 14, 2001 | Sr. Lecturer |
| Do | April 15, 2001 – Oct 04, 2005 | Reader |
| University of Calcutta | Oct 05, 2005– Dec 31, 2005 | Reader |
| University of Calcutta | Jan 01, 2006– Oct 31, 2012 | Associate Professor |
| University of Calcutta | Nov 01, 2012 – Till date | Professor |

8. **Research interests**:

*Please cite briefly the areas of research interests*

- Molecular electronic Structure Theory
- Electronic Non-adiabatic Interactions

9. **Research guidance** :

Number of researchers awarded M.Phil/ Ph.D degrees : …One (Ph.D.)

Number of researchers pursuing M.Phil/ Ph.D : …… Two(Ph.D.)

10. **Projects :**

***Completed projects :2***

| | | |
|---|---|---|
| Structure and photodynamics of small polyatomics.*(Vide:*2009/37/42/BRNS) | Board of Research in Nuclear Sciences (BRNS), India. | 2009-2012 |
| Study of role of exciton and vibronic interaction in NLO properties .. (vide: Conv/002/Nano RAC(2008)) | Centre for Research in Nanoscience & Nanotechnology, University of Calcutta | 2009-2010 |

***Current projects : Nil***

11. **Select list of publications**:

a) ***Journals:***

1. Topological effects in low-lying electronic states of linear $N_2H_2^+$ and $HBNH^+$ associated with onset of bending,
   A.Das, R.Mondal and **D.Mukhopadhyay**
   Molecular Physics **116**, 2642-2651 (2018)
2. Topological study of the $H_3^{++}$ molecular system : $H_3^{++}$ as a cornerstone for building molecules during the Big Bang,
   B.Mukherjee, **D.Mukhopadhyay,** S.Adhikari and M.Baer
   Molecular Physics **116**, 2435-2448 (2018)
3. Conical intersections and diabatic potential energy surfaces for the three lowest electronic singlet states of $H_3^+$,
   S. Mukherjee, **D.Mukhopadhyay** and S.Adhikari
   J Chem. Phys. **141**, 204306 (2014)
4. Study of Nonadiabatic Effects in Low-Lying Electronic States of HCNH with Implication in Its Dissociation to HCN and HNC,
   A. Das and **D. Mukhopadhyay**,
   J. Phys. Chem. **117,**8680-8690(2013).
5. Jahn–Teller intersections involving excited states of the F + $H_2$ system: Identification and influence on the reaction system,
   A. Das and **D. Mukhopadhyay,**
   Chem. Phys. **412**, 51 (2013)
6. Jahn−Teller Intersections Induced by Introduction of Bending in Linear Polyatomics: Study with HCNH, a Selected Molecular System,
   A. Das and **D. Mukhopadhyay**,
   J. Phys. Chem. A **116**, 1774-1785 (2012)
7. The Adiabatic-to-Diabatic Transformation Angle and Topological Phases for Strongly Interacting States: Solution with Four States,
   A.Das and **D. Mukhopadhyay,**
   Int. J. Quan. Chem. **112,** 2767 (2012)
8. Dressed adiabatic and diabatic potentials to study conical intersections for F + $H_2$,
   A. Das, T. Sahoo, **D. Mukhopadhyay**, S. Adhikari, and M. Baer,
   J. Chem. Phys. **136**, 054104 (2012).
9. A tri-atomic Renner-Teller system entangled with Jahn-Teller conical intersections,
   A. Csehi, A. Bende, G. J. Halász, Á. Vibók, A. Das, **D.Mukhopadhyay** and M.Baer
   J. Chem. Phys. 138, 024113 (2013)

**10.** Dressed Adiabatic and Diabatic Potentials for the Renner−Teller/Jahn−Teller F + $H_2$ System,
A. Csehi, A. Bende, G. J. Halász, Á. Vibók, A. Das, **D.Mukhopadhyay**, S.Mukherjee, S.Adhikari and M.Baer , J. Phys. Chem. **117,** 8497-8505 (2013)

**11.** The Adiabatic-to-Diabatic Transformation Angle and the Berry Phase for Coupled Jahn–Teller/Renner–Teller Systems: The F + $H_2$ as a Case Study,
A.Das, **D. Mukhopadhyay**, S. Adhikari, and M. Baer.
Int. J. Quan. Chem. **112,** 2561 (2012).

**12.** Diabatization of the reactive F + $H_2$ system employing rigorous Berry phases,
A.Das**, D. Mukhopadhyay**, S. Adhikari, and M. Baer,
Eur. Phys. J. D **65**, 373 (2011).

**13.** Derivation of diabatic potentials for F + $H_2$ employing non-adiabatic coupling terms,
A.Das, **D. Mukhopadhyay**, S. Adhikari, and M. Baer,
Chem. Phys. Lett. 517, 92 (2011).

**14.** Conical intersections in 22E states of Na3 cluster
A.K. Paul, S. Ray**, D. Mukhopadhyay**, and S. Adhikari ,
Chem. Phys. Lett. **508** (2011) 300–305

**15.** Ab initio calculations on the excited states of Na3 cluster to explore beyond Born-Oppenheimer theories: Adiabatic to diabatic potential energy surfaces and nuclear dynamics.
A.K. Paul, S. Ray**, D. Mukhopadhyay**, and S. Adhikari ,
Journal of Chemical Physics **135**, 034107 (2011)

**16.** Renner–Teller intersections along the collinear axes of polyatomic molecules: $H_2CN$ as a case study,
A. Das, **D. Mukhopadhyay**, S. Adhikari, and M. Baer,
J. Chem. Phys. **133**, 084107 (2010).

**17.** Photodissociation of H2+ upon Exposure to an Intense Pulsed Photonic Fock State
A.K. Paul, S.Adhikari, **D. Mukhopadhyay**, G. J. Halasz, A. Vibok, R. Baer, and M. Baer
J. Phys. Chem. A, **113**, 7331–7337 (2000)

**18.** Applications of linear response theories to compute the low-lying potential energy surfaces: state specific MRCEPA-based approach.
S. Chattopadhyay and **D. Mukhopadhyay**,
J. Phys. B: At. Mol. Opt. Phys. **40**, 1787-1799 ( 2007)

**19.** Stark Profiles of singlet excitons in conjugated polymers
Z.G. Soos, **D. Mukhopadhyay,** M.H. Hennessy
Chem. Phys. **210**, 249-257 (1996)

**20.** Nonlinear optical and electroabsorption spectra of polydiacetylene crystals and films.
**D. Mukhopadhyay** and Z.G. Soos,
J. Chem. Phys. **104**, 1600-1610 (1996).

**21.** Infrared intensity and charge transfer in hydrogen dimmers.
Z.G. Soos, **D. Mukhopadhyay.**
Chem. Phys. Lett. **245**, 194-200 (1995).

**22.** Molecular-exciton approach to spin-charge crossovers in dimerized Hubbard and excitonic chains. **D. Mukhopadhyay**, G.W.Hayden and Z.G. Soos,
Physical Review B **51,** 9476-9492 (1995)

**23.** Vibronic analysis of overlapping resonances and the third-harmonic-generation spectrum of β-carotene. Z.G. Soos and **D. Mukhopadhyay,**
J. Chem.Phys. **101,** 5515-5522 (1994)

**24.** Consistent propagator theory based on the extended coupled-cluster parametrization of the ground state.
B.Dutta, **D. Mukhopadhyay** and D.Mukherjee,
Physical Review A **47**, 3632-3648 (1993).

**25.** The construction of a size-extensive intermediate Hamiltonian in a coupled-cluster framework.
**D. Mukhopadhyay**, B.Dutta(nee Kundu) and D.Mukherjee,
Chem. Phys. Lett. **197**, 236-242 (1992).

**26.** Molecular Applications of size-extensive quasi-Hilbert abd quasi-Fock-space coupled-cluster formalisms using incomplete model spaces.
**D.Mukhopadhyay** and D.Mukherjee,
Chem. Phys. Lett. **177**, 441-446 (1991).

**27.** Aspects of separability in the coupled-cluster based direct methods for energy differences.
**D.Mukhopadhyay**, S.Mukhopadhyay, R.Chaudhuri and D.Mukherjee,
Theor. Chim. Acta **80**, 441-467 (1991).

**28.** A comparative study of core-extensive and core-valence-extensive coupled-cluster theories for energy differences : excitation energies.
S.K.Mukhopadhyay, R. Chaudhuri, **D.Mukhopadhyay** and D.Mukherjee,
Chem. Phys. Lett. **173**, 181-186 (1990)

**29.** A new nonperturbative theory of core-hole ionizations: a compact cluster-expansion technique for treating relaxation effects.
**D.Mukhopadhyay**, R.Chaudhuri and D.Mukherjee,
Chem. Phys. Lett. **172**, 515-521 (1990).

**30.** Size-extensive effective Hamiltonian formalisms using quasi-Hilbert and quasi-Fock space strategies with incomplete model spaces.
**D.Mukhopadhyay** and D.Mukherjee,
Chem. Phys. Lett. **163**, 171-177 (1989).

**31.** Applications of open-shell coupled-cluster theory using an eigenvalue-independent partitioning technique : approximate inclusion of triples in IP calculations.
R.Chaudhuri, **D.Mukhopadhyay** and D.Mukherjee,
Chem. Phys. Lett. **162**, 393-398 (1989)

b) ***Books/ book chapters :***

1. Correlations in Conjugated polymers.
   Z.G.Soos, M.H.Hennessy and **D. Mukhopadhyay,** in "Primary photoexcitations in conjugated polymers : Molecular exciton versus semiconductor band model" pages 1-19, (Ed: N.Serdar Sariciftici, World Scientific Publishing Company, 1998).
2. Π-electron models of conjugated polymers : vibrational and nonlinear optical spectra.
   Z.G.Soos, **D. Mukhopadhyay,** A.Painelli and A.Girlando in "Handbook of Conducting Polymers" 2nd Edition, pages 165-195 (Ed: T.A.Skotheim, R.L.Elsenbaumer and J.R.Reynolds; Marcel Dekker, New York, 1998).
3. Model Hamiltonians for Nonlinear Optical Properties of Conjugated Polymers. Z.G. Soos, **D. Mukhopadhyay** and S.Ramasesha in "Nonlinear Optical Materials" chapter 11, pages 189-210 ( ACS Symposium Series, vol.628; American Chemical Society, 1996)
4. On the construction of size-extensive effective Hamiltonians in general model spaces using quasi-Hilbert and quasi-Fock strategies,
   **D.Mukhopadhyay** and D.Mukherjee, in "Applied many-body methods in spectroscopy and electronic structure" pages 261-284 (Ed: D.Mukherjee, Springer, 1992).
5. An explicitly connected many-body perturbation theory for incomplete model space.
   **D.Mukhopadhyay** and D.Mukherjee, in "Aspects of many-body effects in molecules and extended systems" pages 165-183 (Lecture Notes in Chemistry, Vol.50, Springer Verlag, 1989).

c) ***Conference/ seminar volumes***:

1. Equilibration and Release from deep sites in a Gaussian distribution.
   Z.G. Soos, S.J. Schmidt and **D. Mukhopadhyay** in "Organic Photoreactive Materials and Xerographic Photoreceptors" pages 147-158 ( SPIE - Proceedings of The International Society for Optical Engineering, Vol. 2850, 1996, Ed : S.Ducharme and J.W. Stasiak).
2. Vibronic analysis of π-electronic excitations and polymer fluorescence.
   Z.G. Soos, **D. Mukhopadhyay.** Pages 1125-1137, in Proceedings of 27th International SAMPE Technical Conference, Oct 9 -12, 1995, Vol.27 (Eds: R.J.Martinez, H.Arris, J.A. Emerson, G.Pike).

3. Vibronic analysis of NLO spectra of PDA crystals and films. **D. Mukhopadhyay** and Z.G. Soos, in "Optical and Photonic Applications of Electroactive and Conducting Polymers" pages 116-127 ( SPIE - Proceedings of The International Society for Optical Engineering, Vol. 2528, 1995, Ed : S.C.Yang and P.Chandrasekhar).

d) ***Other publications*** :

1. arXiv:0911.5010
   Are all Quasi-static Processes Reversible?
   Debasis Mukhopadhyay, Kamal Bhattacharyya
   Comments: 11 pages; Subjects: Chemical Physics (physics.chem-ph); Statistical Mechanics (cond-mat.stat-mech)

12. **Membership of Learned Societies**: Life member, IACS
13. **Patents : Nil**
14. **Invited lectures delivered : In 2016 :** One in a National Symposium in Burdwan University, Burdwan, W.B.
15. **Awards : Nil**
16. **Other notable activities** : Post-doctoral Research/Visiting Scientist
    a) 2007 : Visiting Hebrew University and participating in a symposium in Eilat, Israel
    b) 1998 : Visiting Institute of Molecular Science, Japan
    c) 1994-1996 : Post doctoral research in Chemistry Department, Princeton University, USA