Bikramaditya Mandal, Ph.D.

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EMPLOYMENT

Postdoctoral researcher

1. **University of Nevada** *(with Prof. Balakrishnan Naduvalath)* Las Vegas, NV, *January 2023 ─ Now*
   Major Projects:
   - Stereodynamics of controlled collisions of HD + D_2, HD/D_2 + He, D_2 + Ne in the cold energy regime
   - Reactive scattering of $Li^7 + Li_2^6$ in the ultracold energy regime

2. **Marquette University** *(with Prof. Dmitri Babikov)* Milwaukee, WI, *May 2021 ─ Dec 2022*
   Major Projects:
   - Mixed Quantum/Classical theory (MQCT) for collisional quenching of PAHs in the interstellar media
   - Thermally averaged rotational rate coefficients for collisions of H_2O + H_2O for astronomical modeling

EDUCATION

Marquette University Milwaukee, WI
Ph.D. *August 2016 ─ May 2021*
Dissertation: "Development of MQCT Method for Calculations of Collisional Energy Transfer for Astrochemistry and Planetary Atmospheres." (Advisor: Dr. Dmitri Babikov)
Major Projects:
- Adiabatic trajectory approximation within the MQCT framework
- Calculations of differential cross-sections using MQCT
- User-ready program for calculations of inelastic scattering of two molecules

Visva-Bharati University Santiniketan, India
M.Sc. in Chemistry *(Specialization: Physical Chemistry)* *2013 ─ 2015*
Thesis title: "The role of interplay between the potential and ambient energies on the vibration energy harvesting." (Advisor: Dr. Bidhan Chandra Bag)

Visva-Bharati University Santiniketan, India
B.Sc. (Major: Chemistry) *2010 ─ 2013*
Minor: Physics & Mathematics

PUBLICATIONS

1. Sanz-Sanz C.[†], **Mandal B.**[†], Jambrina P., Aoiz J., Naduvalath B., Cold collisions of highly vibrationally excited and aligned D_2 with Ne, ([†]contributed equally) *J. Chem. Phys.*, 2024 (under review).
2. **Mandal B.**, Patkowski K., Jambrina P., Aoiz J., Naduvalath B., Cold collisions of stereodynamically prepared HD and D_2 with He, *J. Chem. Phys.*, 2024 (accepted; waiting for proof).
3. Joy C., Bostan D., **Mandal B.**, Babikov D., Rate coefficients for rotational state-to-state transitions in H_2O + H_2 collisions as predicted by mixed quantum/classical theory, *Astron. & Astrophys*, 692, A229, 2024.
4. Bostan D., **Mandal B.**, Babikov D., On mixed quantum/classical theory for rotationally inelastic scattering of identical collision partners *Phys. Chem. Chem. Phys.*, 26, 27567, 2024.
5. **Mandal B.**, Żółtowski M., Cordiner M., Lique F., Babikov D., Rotational state-to-state transition rate coefficients for H_2O + H_2O collisions at non-equilibrium conditions, *Astron. & Astrophys*, 688, A208, 2024.

6. **Mandal B.**, Kroft J., Jambrina P., Guo H., Aoiz J., Naduvalath B., Stereodynamical control of cold HD + D_2 collisions, *Phys. Chem. Chem. Phys.*, 26, 18368, 2024.
7. Joy C., **Mandal B.**, Bostan D., Dubernet M. L., Babikov D., Mixed quantum/classical theory (MQCT) approach to the dynamics of molecule-molecule collisions in complex systems. *Faraday Discussions*, 251, 225, 2024.
8. Bostan D., **Mandal B.**, Joy C., Żółtowski M., Lique F., Loreau J., Quintas-Sánchez E., Batista-Planas A., Dawes R., Babikov D., Two potential energy surfaces for CO + CO system: A comparative study using mixed quantum/classical theory of rotationally inelastic scattering. *Phys. Chem. Chem. Phys.* 26, 6627, 2024. (**Published as Cover**)
9. Dubernet M. L. … **Mandal B.** … *et al*. BASECOL2023 scientific content. *Astron. & Astrophys*, 683, A40, 2024.
10. **Mandal B.**, Bostan D., Joy C., Babikov D., MQCT 2024: A program for calculations of inelastic scattering of two molecules. *Comp. Phys. Comm.*, 294, 108938, 2024.
11. **Mandal B.**, Babikov D., Improved temperature dependence of rate coefficients for rotational state-to-state transitions in H_2O + H_2O collisions. *Astron. & Astrophys.*, 678, A51, 2023.
12. Joy C., **Mandal B.**, Bostan D., Babikov D., Mixed quantum/classical theory for rotational energy exchange in symmetric-top-rotor + linear-rotor collisions and a case study of the ND_3 + D_2 system. *Phys. Chem. Chem. Phys.* 25, 17287, 2023.
13. Bostan D., **Mandal B.**, Joy C., Babikov D., Description of quantum interference using mixed quantum/classical theory of inelastic scattering. *Phys. Chem. Chem. Phys.* 25, 15683, 2023.
14. **Mandal B.**, Babikov D., Rate coefficients for rotational state-to-state transitions in H_2O + H_2O collisions for cometary and planetary applications, as predicted by mixed quantum/classical theory. *Astron. & Astrophys.*, 671, A51, 2023.
15. **Mandal B.**, Joy C., Bostan D., Eng A., Babikov D., Adiabatic trajectory approximation – new general method in the toolbox of mixed quantum/classical theory for collisional energy transfer. *J. Phys. Chem. Letters*, 14(3), 817-824, 2023. (**Published as Cover**)
16. **Mandal B.**, Joy C., Bostan D., Babikov D., MQCT – A program for calculations of inelastic scattering of two molecules. *VIRT&L-COMM*, 24 (3), ISSN: 2279-8773, 2022.
    Conference proceedings: http://services.chm.unipg.it/ojs/index.php/virtlcomm/article/view/281/284
17. **Mandal B.**, Joy C., Semenov A., Babikov D., Mixed quantum/classical theory for collisional quenching of PAHs in the interstellar media. *Journal of Earth and Space Chemistry*, 6(3), 521-529, 2022.
18. **Mandal B.**, Semenov A., Babikov D., Adiabatic trajectory approximation within the framework of mixed quantum/classical theory. *J. Phys. Chem. A.*, 124 (47), 9877-9888, 2020.
19. Boursier C., **Mandal B.**, Babikov D., Dubernet M.L., New H_2O-H_2O collisional rate coefficients for cometary applications. *Monthly Notices of the Royal Astronomical Society*, 498 (4), 5489-5497, 2020.
20. Semenov A.,† **Mandal B.**,† Babikov D., MQCT: User-ready program for calculations of inelastic scattering of two molecules. *Comp. Phys. Comm.*, 252, 107155, 2020. (†contributed equally)
21. **Mandal B.**, Semenov A., Babikov D., Calculations of differential cross sections using mixed quantum/classical theory of inelastic scattering. *J. Phys. Chem. A.*, 122 (30), 6157-6165, 2018.
22. Borgohain G., **Mandal B.**, Paul S., Molecular dynamics approach to understand the denaturing effect of a millimolar concentration of dodine on a λ-repressor and counteraction by trehalose. *Phys. Chem. Chem. Phys.* 19 (20), 13160-13171, 2017.
23. Ray S., Mondal S., **Mandal B.**, Bag B. C., The role of interplay between the potential and ambient energies on the vibration energy harvesting. *The Euro. Phys. Jour. B.* 89 (10), 224-236, 2016.

EXPERIENCE IN APPLYING FOR RESEARCH GRANT

- **NASA Postdoctoral Program (NPP) - Goddard Space Flight Center** for the **March 2023** cycle

Status: Pending (The application was reviewed by an external peer review panel and evaluated and ranked with other applicants. It may be reconsidered for an NPP award within the year.)

- **The Molecular Sciences Software Institute (MolSSI)** Fellowship for the 2020-2021 & 2021-2022 cycle

Status: **Not funded** (Application containing research proposal and software development plan was reviewed by MolSSI Science and Software Advisory Board and was encouraged to reapply in the next term.)

SCHOLASTIC ACHIEVEMENTS

- **American Institute of Chemists (AIC) award,** Marquette University, USA 2021
- **Dr. John J. Eisch Fellowship,** Marquette University, USA 2020 – 2021
- **Denis J. O'Brien Summer Fellowship,** Marquette University, USA 2019
- **Merit cum Means Scholarship,** Visva-Bharati University, India 2008 – 2010
- **Swami Vivekananda Merit Scholarship,** West Bengal, India 2007
- **National Means cum Merit Scholarship,** West Bengal, India 2005

TEACHING EXPERIENCE

Computational Chemistry CHE 428-0001 (University of Nevada, Las Vegas) Fall 2023–24 (for 2 weeks)

- Prepared in-class teaching material for the course including, but not limited to, Born-Oppenheimer Approximation, Hartree Self-Consistent-Field (SCF) method, Hartree-Fock
- Taught and helped students to successfully execute computational calculations in class for the application of quantum mechanics within Chemistry subject knowledge
- The major topics covered were geometry and energy optimization, vibrational frequency calculation, building potential energy surface (PES), finding transition state structure and intrinsic reaction coordinates for reaction path. These were accomplished by introducing students to the Chemistry software package Gaussian09
- Taught students to analyze output generated from these calculations using Avogadro (an open-source molecule-building software)
- Prepared and shared required video tutorials for students before attending the course, including, but not limited to, knowledge of using high-performance computing (HPC) clusters, navigating within Unix operating systems (OS) using command line interface (CLI), basic software installation for MacOS, Unix OS, and Windows, and building and visualizing molecules using Chemistry software

General Chemistry 1001, 1002 (Marquette University) Fall 2016, 17, 19 & Spring 2019

Graduate Teaching Assistant

- Conducted weekly recitation sessions.
- Conducted weekly laboratory sessions.
- Conducted weekly office hours.
- Graded homework papers, laboratory reports, quizzes, and examination papers

CONFERENCES & PRESENTATIONS

55th annual meeting of the APS division of atomic, molecular and optical physics Fort Worth, TX 2024

Poster: *"Stereodynamical control of cold HD+D_2 collisions."*

Dynamics of Molecular Collisions XXVII Big Sky, MT 2019

Poster: *"Inelastic scattering of molecules within mixed quantum/ classical theory (MQCT) framework."*

50th annual meeting of the APS division of atomic, molecular and optical physics Milwaukee, WI 2019

Oral: *"Mixed quantum/classical theory (MQCT) to study inelastic scattering of molecules."*

ACS Great Lakes Regional Meeting Chicago, IL 2019

***Oral**: "Mixed quantum/classical study of symmetry-driven isotope effects in the recombination reactions: Application to S_2^* + Ar energy transfer."*
A Celebration of Research in the Klingler College of Arts & Sciences Milwaukee, WI 2019
***Poster**: "Sulfur allotropes: A connection between the past and the future."* (featured in College Magazine)
51st Midwest Theoretical Chemistry Conference Notre Dame, IN 2019
***Poster**: "Symmetry-driven isotope effect in the recombination reaction of S_2^* + Ar energy transfer within mixed quantum/classical theory framework."*
50th Midwest Theoretical Chemistry Conference Chicago, IL 2018
***Poster**: "Calculation of inelastic and elastic differential cross sections within mixed quantum/classical theory framework."*
Milwaukee ACS Conference Milwaukee, WI 2018
***Poster**: "Towards dynamics study of sulfur recombination reactions using mixed quantum/classical theory."*
Forward Thinking Poster Session and Colloquy Milwaukee, WI 2017
***Poster**: "Theoretical/computational studies of energy transfer in molecules relevant to planetary atmospheres."*
49th Midwest Theoretical Chemistry Conference East Lansing, MI 2017
***Poster**: "Calculations of differential cross sections using mixed quantum/classical theory of inelastic scattering."*
Milwaukee ACS Conference Milwaukee, WI 2017
***Poster**: "Calculations of cross sections using mixed quantum/classical theory of rotationally inelastic scattering."*

WORKSHOP

- Practical Quantum Computing: Asynchronous Workshop, 28 June-28 July, QUANTGATES, UK.
- ACCESS HPC Workshop: Machine Learning and BIG DATA, May 23-24, 2023, University of Utah, Salt Lake City, UT.
- American Physical Society (APS) GSNP (Group on Statistical & Nonlinear Physics) short course on Information Theory in Machine Learning and Physics, March 5, 2023, Las Vegas, NV.

DEVELOPED CODE REPOSITORY

- MQCT first release: https://github.com/bikramaditya-mandal/MQCT, http://dx.doi.org/10.17632/sg36r35njz.1
- MQCT 2022: https://github.com/bikramaditya-mandal/MQCT_2022
- MQCT: https://github.com/MarquetteQuantum/MQCT.git https://doi.org/10.17632/sg36r35njz.2

TECHNICAL SKILLS

- **OS**: Linux, MacOS, Windows
- **Programming languages**: Fortran, Python, Unix shells, MATLAB, C
- **AI/ML tools**: TensorFlow, Gaussian Processes (GPR, GPFlow)
- **Quantum Computing tools:** Qiskit, IBM-Quantum, QAOA
- **Numerical tools**: LAPack, MKL, BLAS, ARPACK, PARPACK, Numerical recipes
- **HPC (CPU/Distributed Memory)**: Massage Passing Interface or MPI (MPICH, OpenMPI)
- **HPC (GPU/Shared Memory)**: OpenMP
- **Computational chemistry programs**: Molpro, Gaussian, AMBER
- **Molecular visualization**: VMD, Avogadro, Packmol, GaussView
- **Chemistry software**: Origin, Chemdraw
- **Non-chemistry software**: MS Office, LATEX, Adobe CS Suite, XMGrace