BHASKAR RANA

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CONTACT INFORMATION

Stanford University
Department of Chemistry
SLAC National Accelerator Laboratory
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EDUCATION

2022-Present Postdoctoral Scholar
Stanford University, USA

2016-2022 Doctor of Philosophy (Ph.D.) in Chemistry,
Department of Chemistry and Biochemistry,
The Ohio State University, USA
CGPA: 3.65/4

2014-2016 Master of Science (M.Sc.) in Chemistry
Department of Chemistry,
Indian Institute of Technology Kanpur, India
CGPA: 9.60/10

2011-2014 Bachelor of Science (B.Sc.) in Chemistry,
Department of Chemistry,
University of Calcutta, Kolkata, India
CGPA: 85.5/100

RESEARCH EXPERIENCE

2022-Present Postdoctoral Scholar, Stanford University,
Department of Chemistry,
Advisor: **Prof. Todd J. Martinez and Dr. Edward Hohenstein**

2016-2022 Ph.D. Thesis, The Ohio State University,
Department of Chemistry and Biochemistry,
Advisor: **Prof. John M. Herbert**
Thesis: *Development of QM/MM Techniques to Study the Structure and Spectroscopy of Single Ion and Radical Dynamics Study in Liquid Water.*

January-April 2016 M.Sc. Thesis, Indian Institute of Technology Kanpur
Department of Chemistry,

Advisor: **Prof. Amalendu Chandra**
Thesis: *Theoretical Investigation of Ultrafast IR and Raman Spectra for Different Aqueous Ionic Solutions Using Combined Electronic Structure /Molecular Dynamics Approach.*

May-July 2015 Summer Internship, Indian Institute of Science, Bangalore, India.
Department of Inorganic and Physical Chemistry,
Advisor: **Dr. Atanu Bhattacharya**
Project Title: *Theoretical Investigation of Ultrafast Charge Migration Through Different Systems and Their Dynamics Study.*

May-July 2014 Summer Internship, Indian Institute of Technology Kanpur
Department of Chemistry,
Advisor: **Prof. Sankar Prasad Rath**
Project Title: *Axial Phenoxide Coordination on Di-iron (III) Bisporphyrin: Synthesis and Spectral Characterizations.*

PUBLICATIONS

Graduate Publications

1. **Rana, B.**; Hohenstein, E. G., Martinez, T. J. Controlling photochemistry of molecules inside an optical cavity in the strong-field regime. (In preparation)

2. **Rana, B.**; Herbert, J. M. Correcting π-delocalization error for conformational energies of conjugated molecules using density-corrected DFT. (In preparation)

3. **Rana, B.**; Coons, M. P.; Herbert, J. M. Detection and correction of delocalization errors for electron and hole polarons using density-corrected DFT. *J. Phys. Chem. Lett.* **2022**, 13, 5275-5284.

4. Epifanovsky, E. et al. Software for the frontiers of quantum chemistry: An overview of development in the Q-CHEM 5 package. *J. Chem. Phys.* **2021**, 155, 084801:1-59.

5. **Rana, B.**; Herbert, J. M. Hidden hemibonding in the aqueous hydroxyl radical. *J. Phys. Chem. Lett.* **2021**, 12, 8053-8060.

6. **Rana, B.**; Herbert, J. M. Role of hemibonding in the structure and ultraviolet spectroscopy of the aqueous hydroxyl radical. *Phys. Chem. Chem. Phys.* **2020**, 22, 27829-27844.

7. Dasgupta, S.; **Rana, B.**; Herbert, J. M., *Ab initio* investigation of the resonance Raman spectrum of the hydrated electron. *J. Phys. Chem. B* **2019**, 123, 8074-8085.

8. Liu, J.; **Rana, B.**; Liu, K.-Y.; Herbert, J. M., Variational formulation of the generalized many-body expansion with self-consistent charge embedding: Simple and correct analytic energy gradient for fragment-based *ab initio* molecular dynamics. *J. Phys. Chem. Lett.* **2019**, 10, 3877-3886.

9. Holden, Z. C.; **Rana, B.**; Herbert, J. M. Analytic gradient for the QM/MM-Ewald method using charges derived from the electrostatic potential: Theory, implementation, and application to *ab*

initio molecular dynamics simulation of the aqueous electron. *J. Chem. Phys.* **2019**, 150, 144115:1-20.

Undergraduate Publications

1. Chandra, S.; **Rana, B.**; Periyasamy, G.; Bhattacharya, A. On the Ultrafast Charge Migration Dynamics in Isolated Ionized Halogen, Chalcogen, Pnicogen, and Tetrel Bonded Clusters. *Chem. Phys.* **2016**, *472*, 61-71.

TECHNICAL SKILLS

OS: Linux, Windows
Programming Language: C,C++, Fortran, Python, Unix shells
Computational chemistry packages: Terachem**,** Q-Chem, CP2K, MOLPRO, GROMACS, Gaussian
Molecule visualization: IQmol, Avogadro, VMD
Non-chemistry software: MatLab, LATEX, Adobe Illustrator, Mathematica, Adobe Photoshop

TEACHING EXPERIENCE

The Ohio State University

2016(AU)	Graduate Teaching Assistant, CHEM 1210, Chemistry (*General Chemistry*)
2017(SP)	Graduate Teaching Assistant, CHEM 1210, Chemistry (*General Chemistry*)
2017(AU)	Graduate Teaching Assistant, CHEM 1210, Chemistry (*General Chemistry*)
2018(SP)	Graduate Teaching Assistant, CHEM 4300, Chemistry (*Quantum Chemistry & Kinetics*)
2018(AU)	Graduate Teaching Assistant, CHEM 4300, Chemistry (*Quantum Chemistry & Kinetics*)
2019(SP)	Graduate Teaching Assistant, CHEM 4310, Chemistry (*Statistical Mechanics*)
2020(AU)	Graduate Teaching Assistant, CHEM 6510, Chemistry (*Quantum Mechanics*)
2020(AU)	Graduate Teaching Assistant, CHEM 6540, Chemistry (*Electronic Structure Theory*)

PRESENTATIONS

2022 (July) **Rana, B.**; Hohenstein, E. G..; Martinez, T. J. Controlling photochemistry of molecules inside an optical cavity in the strong-field regime (POSTER). American Conference on Theoretical Chemistry (ACTC), Lake Tahoe, USA.

2021 (April) **Rana, B.**; Herbert, J. M. Role of hemibonding in the structure and ultraviolet spectroscopy of the aqueous hydroxyl radical (ORAL), Physical Chemistry Divisional Seminar, The Ohio State University.

2021 (April) **Rana, B.**; Herbert, J. M. Role of hemibonding in the structure and ultraviolet spectroscopy of the aqueous hydroxyl radical (ORAL) ACS Spring 2021 Conference (Virtual).

2019 (June) **Rana, B.**; Dasgupta, S.; Herbert, J. M. QM/MM-Ewald method using charges derived from electrostatic potential and its application to ab initio molecular dynamics simulation of hydrated electron (POSTER). Midwest Theoretical Chemistry Conference, University of Notre Dame.

2019 (Aug) **Rana, B.**; Dasgupta, S.; Herbert, J. M. QM/MM-Ewald method using charges derived from electrostatic potential and its application to ab initio molecular dynamics simulation of hydrated electron (POSTER). Penn Conference on Theoretical Chemistry (PCTC), University of Pennsylvania.

2016 (April) **Rana, B.**; Das, B.; Chandra, A. Theoretical Investigation of Ultrafast IR and Raman Spectra for different aqueous ionic solutions using combined Electronic Structure / Molecular Dynamics approach (POSTER). M.Sc. Research Presentation, Department of Chemistry, Indian Institute of Kanpur.

AWARDS AND HONORS

2014 **All India rank 23** in National Eligibility Test (**NET**), Chemical Science, Junior Research Fellowship Council of Scientific & Industrial Research, Government of India (50,000 students from around the India appeared for the exam)

2014 **All India rank 3** in Hyderabad Central University (**HCU**) entrance exam for M.Sc. (among 20,000 students in Chemistry from all around the India)

2014 **All India rank 3** in IIT-JAM Joint Admissions entrance exam for M.Sc. (among 20,000 students in Chemistry from all around the India)

2011-2016 **Innovation in Science Pursuit for Inspired Research (INSPIRE) Fellow**, Department of Science and Technology, Government of India
Stipend for undergraduate and master's studies for being top 1% students in 12th grade.

CONFERENCE, MEETINGS, and WORKSHOPS

2017 Midwest Theoretical Chemistry Conference, Michigan State University
2018 Midwest Theoretical Chemistry Conference, University of Chicago
2019 Virtual Winter School on Computational Chemistry
2019 Midwest Theoretical Chemistry Conference, University of Notre Dame
2019 Penn Conference on Theoretical Chemistry (PCTC), University of Pennsylvania.
2021 Virtual Winter School on Computational Chemistry
2021 ACS Spring 2021 Virtual Conference
2021 International Workshop on Recent Developments in Electronic Structure
2021 Telluride School on Theoretical Chemistry
2022 American Conference on Theoretical Chemistry