

Ram S. Bhatta, Ph.D.

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EDUCATION

Ph.D., Chemistry (2008 – 2012), The University of Akron, OH, USA
M. Sc., Chemistry (2000 – 2002), Tribhuvan University, Nepal
B. Sc., Chemistry (1996 – 1999), Tribhuvan University, Nepal

PROFESSIONAL APPOINTMENTS

Lecturer of Chemistry (08/2018 – present), Texas A&M University San Antonio, TX
Adjunct Chemistry Faculty (08/2017 – 08/2018), University of the Incarnate Word, TX
Postdoctoral Research Associate (01/2016 – 12/2016), UNT Health Science Center, TX
Postdoctoral Research Associate (12/2012 – 01/2016), Department of Polymer Science, The University of Akron, OH, USA
Teaching/Research Assistant (01/2008 – 12/2012), Department of Chemistry, The University of Akron, OH, USA
Lecturer of Chemistry (10/2002 – 04/2007, full time); Acme Engineering College, Nepal
Lecturer of Chemistry (07/2002 – 04/2007, part time); REHDON College, Nepal

TEACHING EXPERIENCE

Lecturer of Chemistry (08/2018 - present); Texas A&M University San Antonio, TX

- Teach General Chemistry lectures and laboratories
- Teach Organic Chemistry lectures and laboratories

Adjunct Chemistry Faculty (08/2017 - present); University of the Incarnate Word, TX

- Teach General Chemistry & Chemical Principles lectures and laboratories

Teaching Assistant (01/2008 – 12/2008); The University of Akron, OH, USA

- Taught undergraduate principle of chemistry, qualitative analysis and general organic and biochemistry laboratories

Lecturer of Chemistry (10/2002 – 04/2007, full time); Acme Engineering College, Nepal

- Taught Diploma and Bachelor of Engineering chemistry courses
- Courses covered: Physical and Organic
- Organized workshops to improve teaching-learning process
- Participated in student recruitment and college services
- Counseled students on issues related to carrier development

Lecturer of Chemistry (Jul 2002 – Apr 2007, part time); REHDON College, Nepal

- Taught undergraduate lectures and laboratories
- Course covered: electrochemistry, chemical kinetics, thermodynamics, atomic structures

- Counseled students experiencing difficulties in the course

RESEARCH MENTORING EXPERIENCE

- Mentored *Brandon Yang* (high school student, 2013) to study interfacial properties of water in contact with poly(3-hexylthiophene) (publication: [Chemical Physics Letters, 635 \(2015\) 139](#))
- Mentored *Prasad Iyer* (undergraduate student, 2011) to perform quantum calculations of enthalpy and frequency shift of acid-base complexes (publication: [Modern Physics Letters B, 28 \(2014\) 1430014](#))
- Mentored *Jonathan Martens* (undergraduate student, 2010) to study polythiophene-hydroxylated surface interactions by tri-methylthiophene-water complexes (*first place winner* on research conference, University of Akron, 2011)
- Mentored *Amy Gao* (high school student, 2008) to calculate torsion-inversion surface for protonated methanol (publication: [Journal of Molecular Structure: THEOCHEM, 941 \(2010\) 22](#))

AWARDS AND HONOR

The Dr. Harold G. Cassidy Award in Chemistry, The University of Akron (2011)

Coblentz Society Student Award (2010) (<http://www.coblentz.org/awards/coblentz-student-awards>)

Golden key international honor (2008)

RESEARCH GRANTS

National Science Foundation-Extreme Science & Engineering Discovery Environment DMR140147, “*First-principles studies of interfacial properties in organic solar cells materials*” **PI: Ram S. Bhatta**, Co-PI: Mesfin Tsige, 2015 (100,000 SUs).

National Science Foundation-Extreme Science & Engineering Discovery Environment TG-CHE140067, “*Structure-property relationships in conjugated polymers*” **PI: Ram S. Bhatta**, 2014 (30,000 SUs).

PUBLICATIONS [High school and undergrad students are marked with #]

1. Kun Yang, Xiang Li, Yi-Fan Huang, Ram S. Bhatta, Jiawei Liu, Mesfin Tsige, Chien-Lung Wang, Stephen Z.D.Cheng, Yu Zhu, “Investigation of hydrogen-bonding mediated molecular packing of diketopyrrolopyrrole based donor-acceptor oligomers in the solid state”, [Polymer, 160 \(2019\) 238](#).
2. Haichang Zhang, Kun Yang, Yu-Ming Chen, **Ram S. Bhatta**, Mesfin Tsige, Stephen ZD Cheng, Yu Zhu, “Polymers Based on Benzodipyrrolidone and Naphthodipyrrolidone with Latent Hydrogen-Bonding on the Main Chain”, [Macromolecular Chemistry and Physics, 218 \(2017\) 1600617](#).
3. **Ram S. Bhatta** and Mesfin Tsige, “Understanding structural and electronic properties of dithienyl benzothiadiazole and its complex with C70”, [Polymer, 75 \(2015\) 73](#).

4. Chang Liu, Chao Yi, Kai Wang, Yali Yang, **Ram S. Bhatta**, Mesfin Tsige, Shuyong Xiao, and Xiong Gong, “Single Junction Polymer Solar Cells with over 10% Efficiency by Novel Two-Dimensional Donor-Acceptor Conjugated Copolymer”, [*ACS Applied Materials & Interfaces*, 7 \(2015\) 4928](#).
5. **Ram S. Bhatta**, G. Pellicane and Mesfin Tsige, “Tuning Range-Separated DFT Functionals for Accurate Orbital Energy Modeling of Conjugated Molecules”, [*Computational and Theoretical Chemistry*, 1070 \(2015\) 14](#).
6. Yeneneh Y. Yimer, Brandon Yang[#], **Ram S. Bhatta** and Mesfin Tsige, “Wetting and Interfacial Properties of Water in Contact with Poly(3-hexylthiophene)”, [*Chemical Physics Letters*, 635 \(2015\) 139](#).
7. **Ram S. Bhatta** and Mesfin Tsige, “Structural dependence of Electronic Properties in A-A-D-A-A-Type Organic Solar Cell Material”, [*International Journal of Photoenergy*, 2015 \(2015\) 1](#). (Invited article)
8. **Ram S. Bhatta** and Mesfin Tsige, “Understanding the Effect of Heteroatoms on Structural and Electronic Properties of Conjugated Polymers”, [*Polymer*, 56 \(2015\) 293](#).
9. Mahesh Dawadi, **Ram S. Bhatta** and David S. Perry, “Contrasting patterns of coupling between the CH stretches and the large-amplitude motions in the molecules, CH₂NH₂, CH₂OH₂⁺ and CH₂CH₂·”, [*Chemical Physics Letters*, 624 \(2015\) 53](#). (Editor’s choice)
10. Jiayuan Miao, **Ram S. Bhatta**, Darrell H. Reneker, Mesfin Tsige and Philip L. Taylor, “Molecular Dynamics Simulations of Relaxation in Stretched PVDF Nanofibers”, [*Polymer*, 56 \(2015\) 482](#).
11. **Ram S. Bhatta** and Mesfin Tsige, “Effect of Fluorination on Electronic Properties of Polythiophene-co-benzodithiophenes and their fullerene complexes”, [*ACS Applied Materials & Interfaces*, 6 \(2014\) 15889](#).
12. **Ram S. Bhatta**, Prasad P. Iyer[#], Ali Dhinojwala and Mesfin Tsige, “A Brief Review of Badger-Bauer Rule and Its Validation From a First-principles Approach”, [*Modern Physics Letters B*, 28 \(2014\) 1430014](#) (invited article).
13. He Zhu, Kshitij Jha, **Ram S. Bhatta**, Mesfin Tsige and Ali Dhinojwala, “Molecular structure of poly(methyl methacrylate) surface I: Combination of interface-sensitive infrared-visible sum frequency generation, molecular dynamics simulations, and ab initio calculations”, [*Langmuir*, 30 \(2014\) 11609](#).
14. **Ram S. Bhatta** and Mesfin Tsige, “Chain Length and Torsional Dependence of Exciton Binding Energies in P3HT and PTB7 Conjugated Polymers: A First-Principles Study”, [*Polymer*, 45 \(2014\) 2667](#).
15. **Ram S. Bhatta**, Mesfin Tsige and Devid Perry, “Torsionally-Induced Blue Shift of the

- Band Gap in Poly(3-hexylthiophene)*”, [*Journal of Computational and Theoretical Nanoscience*, 11 \(2014\) 2157.](#)
16. **Ram S. Bhatta**, Devid Perry and Mesfin Tsige, “*Nanostructures and Electronic Properties of High-Efficiency Electron-Donating Polymer*”, [*Journal of Physical Chemistry A*, 117 \(2013\) 12628.](#)
 17. Mahesh B. Dawadi, **Ram S. Bhatta** and Devid Perry, “*Torsion-inversion tunneling patterns in the CH-stretch vibrationally excited states of the G_{12} family of molecules including methylamine*”, [*Journal of Physical Chemistry A*, 117 \(2013\) 13356.](#)
 18. **Ram S. Bhatta**, Yeneneh Yimer, Devid Perry and Mesfin Tsige, “*An Improved Force-field for Molecular Modeling of Poly(3-hexylthiophene)*”, [*Journal of Physical Chemistry B*, 117 \(2013\) 10035.](#)
 19. **Ram S. Bhatta** and David Perry, “*Correlated backbone Torsional Potentials in Poly(3-methylthiophene)*”, [*Computational and Theoretical Chemistry*, 1008 \(2013\) 90.](#)
 20. **Ram S. Bhatta**, Yeneneh Yimer, Mesfin Tsige and David Perry, “*Conformations and Torsional Potentials of Poly (3-hexylthiophene) Oligomers: Density Functional Calculations up to the Dodecamers*”, [*Computational and Theoretical Chemistry*, 995 \(2012\) 36.](#)
 21. **Ram S. Bhatta**, Amy Gao[#] and David S Perry, “*A Comparative Ab Initio Study of Torsion-inversion Coupling in $CH_3CH_2^{\bullet}$, CH_3NH_2 and $CH_3OH_2^+$* ”, [*Journal of Molecular Structure: THEOCHEM*, 941 \(2010\) 22.](#)

RESEARCH PRESENTATIONS

Oral Presentations at American Physical Society

1. **Ram S. Bhatta** and Mesfin Tsige, “*Small Conjugated Molecules: Orbital Energy Modeling Using Tuned Range-Separated Functional*”, American Physical Society March Meeting, March 2-6, 2015, San Antonio, TX, USA. (<http://meeting.aps.org/Meeting/MAR15/Session/G41.6>)
2. He Zhu, Kshitij Tha, **Ram S. Bhatta** Mesfin Tsige and Ali Dhinojwala, “*Molecular structure of poly(methyl methacrylate) surface: Combination of interface-sensitive infrared-visible sum frequency generation, molecular dynamics simulations, and ab initio calculations*”, American Physical Society March Meeting, March 2-6, 2015, San Antonio, TX, USA. (<http://meeting.aps.org/Meeting/MAR15/Session/Z42.14>)
3. Mesfin Tsige and **Ram S. Bhatta**, “*A Quantum Chemical Study of Structural and Electronic Properties of DTBT and DTBT:C70 Complexes*”, American Physical Society March Meeting, March 2-6, 2015, San Antonio, TX, USA. (<http://meeting.aps.org/Meeting/MAR15/Session/F41.7>)

4. Mahesh Dawadi, Bishnu Thapalia, **Ram S. Bhatta** and David Perry, “*Vibrational Conical Intersections: Implications for Ultrafast Vibrational Dynamics*”, American Physical Society March Meeting, March 2-6, 2015, San Antonio, TX, USA.
(<http://meeting.aps.org/Meeting/MAR15/Session/B26.7>)
5. **Ram S. Bhatta**, David Perry and Mesfin Tsige, “*First principles calculations of conformational and electronic properties of PTB7*”, American Physical Society March Meeting, March 3-7, 2014, Denver, CO, USA.
(<http://meetings.aps.org/Meeting/MAR14/Session/S1.9>)
6. **Ram S. Bhatta**, David Perry and Mesfin Tsige, “*First principles calculations of conformational and electronic properties of PTB7*”, American Physical Society March Meeting, March 3-7, 2014, Denver, CO, USA.
(<http://meetings.aps.org/Meeting/MAR14/Session/S1.9>)
7. Jiayuan Miao, **Ram S. Bhatta**, Christian Kisielowski, Dinesh Lolla, Darrell Reneker, Mesfin Tsige and Philip Taylor, “*Molecular dynamics simulations of electron irradiated PVDF nanofibers*”, American Physical Society March Meeting, March 3-7, 2014, Denver, CO, USA.
(<http://meetings.aps.org/Meeting/MAR14/Session/F21.4>)
8. Mesfin Tsige, **Ram S. Bhatta** and Ali Dhinojwala, “*First principles calculations of enthalpy and O-H stretching frequency of hydrogen-bonded acid-base complexes*”, American Physical Society March Meeting, March 3-7, 2014, Denver, CO, USA.
(<http://meetings.aps.org/Meeting/MAR14/Session/J2>)
9. **Ram S. Bhatta**, Mesfin Tsige and David Perry, “*Frontier Orbital Energy Change of Poly(3-hexylthiophene) oligomers: Effect of Large Amplitude Torsional Motion*”, American Physical Society March Meeting-2013, Baltimore.
(<http://meetings.aps.org/Meeting/MAR13/Event/187921>)
10. **Ram S. Bhatta**, Yeneneh Yimer, David Perry and Mesfin Tsige, “*An Improved Force-field for Molecular Modeling of Crystalline Poly(3-hexylthiophene)*”, American Physical Society March Meeting-2012, Boston.
(<http://meetings.aps.org/Meeting/MAR12/Event/163128>)
11. **Ram S. Bhatta**, Yeneneh Yimer, Mesfin Tsige and David Perry, “*Conformational Dependence of Charge Transport and Band Gap in Poly (3-Hexyl Thiophene) Oligomers*”, American Physical Society Spring Meeting, 2011.
(<http://meeting.aps.org/Meeting/OSS11/Event/150093>)
12. **Ram S. Bhatta** and David S Perry, “*Ab Initio Torsion-Wag Surface for the Ethyl Radical*”, American Physical Society March Meeting, 2009.
(<http://meetings.aps.org/Meeting/MAR09/Event/98948>)

Oral Presentations at International Symposium on Molecular Spectroscopy

13. **Ram S. Bhatta**, Mahesh B. Dawadi and David Perry, “Coupling of the C-H stretch to

- large-amplitude torsion and inversion motions: comparison of CH_3CH_2 , CH_3OH_2^+ and CH_3NH_2^+ , International Symposium on Molecular Spectroscopy, OSU, Columbus, June, 2013. [<https://molspect.chemistry.ohio-state.edu/symposium/Program/RH.html>] (Abstract #RH02)]
14. **Mahesh B. Dawadi, Ram S. Bhatta** and David Perry, “*Torsion-inversion tunneling patterns in the CH-stretch vibrationally excited states of the G_{12} molecules*”, International Symposium on Molecular Spectroscopy, OSU, Columbus, June, 2013. [<https://molspect.chemistry.ohio-state.edu/symposium/Program/RH.html>] (Abstract #RH01)]
15. **Ram S. Bhatta**, Yeneneh Yimer, Mesfin Tsige and David Perry, “*Inter-ring and Hexyl Chain Torsional Potentials in Poly (3-hexylthiophene) Oligomers*”, International Symposium on Molecular Spectroscopy, OSU, Columbus, June, 2011. [https://molspect.chemistry.ohio-state.edu/symposium_66/symposium/Program/RE.html](Abstract #RE01)]
16. **Ram S. Bhatta** and David Perry, “*Comparative Torsion-Inversion Dynamics for CH_3CH_2 , CH_3OH_2^+ and CH_3NH_2* ”, International Symposium on Molecular Spectroscopy, OSU, Columbus, June, 2011. [https://molspect.chemistry.ohio-state.edu/symposium_66/symposium/Program/TB.html] (Abstract #TB10)]
17. **Ram S. Bhatta** and David S Perry, “*Electronic Structure Calculation of Inner-ring Torsional Potentials of Regioregular Poly (3-methyl Thiophene)*”, International Symposium on Molecular Spectroscopy, OSU, Columbus, June, 2010. [https://molspect.chemistry.ohio-state.edu/symposium_65/symposium/Program/TA.html](Abstract #TA07)]
18. **Ram S. Bhatta**, Amy Gao and David S Perry, “*Nature of Torsion-inversion Coupling in CH_3CH_2 , CH_3NH_2 and CH_3OH_2^+* ”, International Symposium on Molecular Spectroscopy, OSU, Columbus, June, 2009. [https://molspect.chemistry.ohio-state.edu/symposium_64/symposium/Program/FB.html] (Abstract #FB04)]

PROFESSIONAL ACTIVITIES

- American Chemical Society (JPC reviewer)
- Royal Society of Chemistry (Analyst reviewer)
- Springer publications (NRL reviewer)
- American Physical Society (member since 2009)