

Isuru R. Ariyaratna

Education

- 2015 – 2021 PhD in Theoretical Chemistry (*Department of Chemistry and Biochemistry, Auburn University, AL 36849, USA*)
- 2009 – 2014 BS Chemistry (*Department of Chemistry, University of Peradeniya, Sri Lanka*)

Professional Employments

- 2021 – Now Postdoctoral Associate (*Department of Chemical Engineering, Massachusetts Institute of Technology, MA 02139, USA*)
- 2020 – 2021 Graduate Research Assistant (*Department of Chemistry and Biochemistry, Auburn University, AL 36849, USA*)
- 2015 – 2020 Graduate Research Assistant (*Department of Chemistry and Biochemistry, Auburn University, AL 36849, USA*)
- 2014 – 2015 Teaching Assistant (*Department of Chemistry and Department of Pharmacy, University of Peradeniya, Sri Lanka*)

Research Experience

- 2021 – Now Development of machine learning models for correlated systems (*Advisor: Prof. Heather J. Kulik*)
- 2016 – 2021 First principle studies on ground and excited electronic states of molecules (*Advisor: Prof. E. Miliordos*)
- 2014 – 2015 Extension of coarse-grained force field to triglycerides (*Advisor: Prof. R. J. K. U. Ranatunga*)
- 2013 – 2014 Nutrients and pharmaceutical ingredients encapsulation by proteins to be used as slow release carriers (*Advisor: Prof. D. N. Karunaratne*)

Research Awards and Distinctions

13. “CCG Research Excellence Award” from the ACS COMP Division Fall 2021.
12. “2021 Outstanding International Student Award” at Auburn University.
11. “NERSC AY 2020–2021 DOE Mission Science Allocation Award” for the proposal titled “Electronic structure analysis of ground and excited states of superatomic superalkalis”.
10. “2020–2021 Harry Merriwether Fellowship” at Auburn University.
9. “2020 Graduate Research and Travel Fellowship” at Auburn University.

8. “2019 Dow Fellowship in Chemistry” at Auburn University.
7. “2018–2019 Dean’s Research Award for PhD Student” at Auburn University.
6. “2018–2019 Outstanding Doctoral Student Award” at Auburn University.
5. “Advancing Science Conference Grant” NOBCChE 2019 St. Louis, MO.
4. “Outstanding Poster Award” at 2018 Southeastern Theoretical Chemistry Association Meeting at Louisiana State University.
3. “COSAM College Specific Best Poster Award” at 2018 This is Research Student Symposium at Auburn University.
2. “2015 Sri Lankan NRC Merit Award” for research.
1. “Best Paper Award” at the “International Research Symposium on Engineering Advancements 2015”.

Scholarly Contributions in Peer-Reviewed Journals

27. Isuru R. Ariyaratna and E. Miliordos, Radical abstraction vs. oxidative addition mechanisms for the activation of the S–H, O–H, and C–H bonds using early transition metal oxides. *Phys. Chem. Chem. Phys.* **23**, 1437–1442 (2021).
DOI: [10.1039/D0CP05513A](https://doi.org/10.1039/D0CP05513A)
26. G. Liu, Isuru R. Ariyaratna, S. M. Ciborowski, Z. Zhu, E. Miliordos, K. H. Bowen, Simultaneous Functionalization of Methane and Carbon Dioxide Mediated by Single Platinum Atomic Anions. *J. Am. Chem. Soc.* **142**, 21556–21561, (2020).
DOI: [10.1021/jacs.0c11112](https://doi.org/10.1021/jacs.0c11112)
25. Isuru R. Ariyaratna and E. Miliordos, Be–Be Bond in Action: Lessons from the Beryllium–Ammonia Complexes $[\text{Be}(\text{NH}_3)_{0-4}]_2^{0,2+}$. *J. Phys. Chem. A.* **124**, 9783–9792 (2020): *Editors’ choice as the cover in the issue.*
DOI: [10.1021/acs.jpca.0c07939](https://doi.org/10.1021/acs.jpca.0c07939)
24. Isuru R. Ariyaratna and E. Miliordos, Geometric and electronic structure analysis of calcium water complexes with one and two solvation shells. *Phys. Chem. Chem. Phys.* **22**, 22426–22435 (2020).
DOI: [10.1039/D0CP04309E](https://doi.org/10.1039/D0CP04309E)
23. Isuru R. Ariyaratna, E. Miliordos, *Ab initio* investigation of the ground and excited states of ZrO^+ and NbO^+ . *J. Quant. Spectrosc. Ra.* **255**, 107265 (2020).
DOI: [10.1016/j.jqsrt.2020.107265](https://doi.org/10.1016/j.jqsrt.2020.107265)
22. Isuru R. Ariyaratna, Nuno M. S. Almeida, E. Miliordos, *Ab initio* investigation of the ground and excited states of $\text{RuO}^{+,0,-}$ and their reaction with water. *Phys. Chem. Chem. Phys.* **22**, 16072–16079 (2020).
DOI: [10.1039/D0CP02468F](https://doi.org/10.1039/D0CP02468F)
21. Isuru R. Ariyaratna, Filip Pawłowski, Joseph Vincent Ortiz, E. Miliordos, Aufbau Principle for Diffuse Electrons of Double-Shell Metal Ammonia Complexes: The Case of $\text{M}(\text{NH}_3)_4@12\text{NH}_3$, $\text{M}=\text{Li}, \text{Be}^+, \text{B}^{2+}$. *J. Phys. Chem. A.* **124**, 505–512 (2020): *Editors’ choice as the cover in the issue.*
DOI: [10.1021/acs.jpca.9b07734](https://doi.org/10.1021/acs.jpca.9b07734)
20. Isuru R. Ariyaratna, E. Miliordos, Carbon monoxide activation by atomic thorium: ground and excited state reaction pathways. *Phys. Chem. Chem. Phys.* **21**, 24469–24477 (2019): *A PCCP Hot Article.*
DOI: [10.1039/C9CP04946K](https://doi.org/10.1039/C9CP04946K)
19. Nuno M. S. Almeida, Isuru R. Ariyaratna, E. Miliordos, O–H and C–H Bond Activation of Water and Methane by RuO^{2+} and $(\text{NH}_3)\text{RuO}^{2+}$: Ground and Excited States. *J. Phys. Chem. A.* **123**, 9336–9344

- (2019).
DOI: [10.1021/acs.jpca.9b05910](https://doi.org/10.1021/acs.jpca.9b05910)
18. Isuru R. Ariyaratna, Nuno M. S. Almeida, E. Miliordos, Stability and Electronic Features of Calcium Hexa-, Hepta- and Octa-Coordinated Ammonia Complexes: A First Principles Study. *J. Phys. Chem. A.* 123, 6744–6750 (2019).
DOI: [10.1021/acs.jpca.9b04966](https://doi.org/10.1021/acs.jpca.9b04966)
 17. Isuru R. Ariyaratna, E. Miliordos, Superatomic nature of alkaline earth metal–water complexes: the cases of $\text{Be}(\text{H}_2\text{O})_4^{0,+}$ and $\text{Mg}(\text{H}_2\text{O})_6^{0,+}$. *Phys. Chem. Chem. Phys.* 21, 15861–15870 (2019).
DOI: [10.1039/C9CP01897B](https://doi.org/10.1039/C9CP01897B)
 16. G. Liu, Z. Zhu, S. M. Ciborowski, Isuru R. Ariyaratna, E. Miliordos, K. H. Bowen, Selective Activation of the C–H Bond in Methane by Single Platinum Atomic Anions. *Angew. Chem. Int. Ed.* 58, 7773–7777 (2019).
DOI: [10.1002/anie.201903252](https://doi.org/10.1002/anie.201903252)
 15. Isuru R. Ariyaratna, E. Miliordos, Electronic and geometric structure analysis of neutral and anionic metal nitric chalcogens: The case of MNX series (M=Li, Na, Be and X = O, S, Se, Te) *J. Comput. Chem.* 40, 1740–1751 (2019): *Editors' choice as the cover in the issue.*
DOI: [10.1012/jcc.25829](https://doi.org/10.1012/jcc.25829)
 14. A. Kalemios, Isuru R. Ariyaratna, Shahriar N. Khan, E. Miliordos, A. Mavridis, “Hypervalency” and the Chemical Bond. *Comput. Theor. Chem.* 1153, 65–74 (2019).
DOI: [10.1016/j.comptc.2019.02.014](https://doi.org/10.1016/j.comptc.2019.02.014)
 13. Isuru R. Ariyaratna, E. Miliordos, Electronic and geometric structure analysis of neutral and anionic alkali metal complexes of the CX series (X = O, S, Se, Te, Po): The case of $\text{M}(\text{CX})_{n=1-4}$ (M = Li, Na) and their dimers. *J. Comput. Chem.* 40, 1344–1351 (2019): *Editors' choice as the cover in the issue.*
DOI: [10.1002/jcc.25791](https://doi.org/10.1002/jcc.25791)
 12. Isuru R. Ariyaratna, Filip Pawłowski, Joseph Vincent Ortiz, E. Miliordos, Molecules mimicking atoms: monomers and dimers of alkali metal solvated electron precursors. *Phys. Chem. Chem. Phys.* 20, 24186–24191 (2018).
DOI: [10.1039/c8cp05497e](https://doi.org/10.1039/c8cp05497e)
 11. Isuru R. Ariyaratna, E. Miliordos, Dative bonds versus electron solvation in tri-coordinated beryllium complexes: $\text{Be}(\text{CX})_3$ [X=O, S, Se, Te, Po] and $\text{Be}(\text{PH}_3)_3$ versus $\text{Be}(\text{NH}_3)_3$. *Int. J. Quantum Chem.* 118(18), 1–8 (2018): *Editors' choice as the cover in the issue.*
DOI: [10.1002/qua.25673](https://doi.org/10.1002/qua.25673)
 10. Nuno M. S. Almeida, Isuru R. Ariyaratna, E. Miliordos, *Ab initio* calculations on the ground and excited electronic states of neutral and charged palladium monoxide, $\text{PdO}^{0,+,-}$. *Phys. Chem. Chem. Phys.* 20, 14578–14586 (2018).
DOI: [10.1039/C8CP01251B](https://doi.org/10.1039/C8CP01251B)
 9. Isuru R. Ariyaratna, E. Miliordos, *Ab initio* investigation of the ground and excited states of $\text{MoO}^{+,2+,-}$ and their catalytic strength on water activation. *Phys. Chem. Chem. Phys.* 20, 12278–12287 (2018).
DOI: [10.1039/c8cp01676c](https://doi.org/10.1039/c8cp01676c)
 8. Isuru R. Ariyaratna, Shahriar N. Khan, Filip Pawłowski, Joseph Vincent Ortiz, E. Miliordos, Aufbau Rules for Solvated Electron Precursors: $\text{Be}(\text{NH}_3)_4^{0,\pm}$ Complexes and Beyond. *J. Phys. Chem. Lett.* 9, 84–88 (2017).
DOI: [10.1021/acs.jpcclett.7b03000](https://doi.org/10.1021/acs.jpcclett.7b03000)
 7. E. E. Hardy, K. M. Wyss, J. D. Gorden, Isuru R. Ariyaratna, E. Miliordos, A. E. V. Gorden, Th(IV) and

- Ce(IV) naphthylsalophen sandwich complexes: characterization of unusual thorium fluorescence in solution and solid–state. *Chem. Commun.* 53, 11984–11987 (2017): *Editors' choice as the cover in the issue.*
DOI: [10.1039/C7CC06868A](https://doi.org/10.1039/C7CC06868A)
6. Isuru R. Ariyaratna, E. Miliordos, The Versatile Personality of Beryllium: Be(O₂)_{1–2} vs Be(CO)_{1–2}. *J. Phys. Chem. A.* 121, 7051–7058 (2017).
DOI: [10.1021/acs.jpca.7b06519](https://doi.org/10.1021/acs.jpca.7b06519)
 5. Isuru R. Ariyaratna*, R. M. P. I. Rajakaruna, D. N. Karunaratne, The rise of inorganic nanomaterial implementation in food applications. *Food Control.* 77, 251–259 (2017).
DOI: [10.1016/j.foodcont.2017.02.016](https://doi.org/10.1016/j.foodcont.2017.02.016)
 4. Isuru R. Ariyaratna, D. N. Karunaratne, Microencapsulation stabilizes curcumin for efficient delivery in food applications. *Food Packag. Shelf Life.* 10, 79–86 (2016).
DOI: [10.1016/j.fpsl.2016.10.005](https://doi.org/10.1016/j.fpsl.2016.10.005)
 3. R. M. P. I. Rajakaruna, Isuru R. Ariyaratna, D. Nedra Karunaratne, Challenges and strategies to combat global iron deficiency by food fortification. *Ceylon J. Sci.* 45 (2), 3–14 (2016).
DOI: [10.4038/cjs.v45i2.7384](https://doi.org/10.4038/cjs.v45i2.7384)
 2. D. N. Karunaratne, Isuru R. Ariyaratna, D. Welideniya, A. Siriwardene, D. Gunasekara, V. Karunaratne, Nanotechnological Strategies to Improve Water Solubility of Commercially Available Drugs. *Curr. Nanomed.* 7, 84–110 (2016): *Editors' Choice Article.*
DOI: [10.2174/2468187307666161227171349](https://doi.org/10.2174/2468187307666161227171349)
 1. Isuru R. Ariyaratna, D. N. Karunaratne, Use of chickpea protein for encapsulation of folate to enhance nutritional potency and stability. *Food Bioprod. Process.* 95, 76–82 (2015).
DOI: [10.1016/j.fbp.2015.04.004](https://doi.org/10.1016/j.fbp.2015.04.004)

Contribution for Book Chapters

3. R. M. P. I. Rajakaruna, Isuru R. Ariyaratna*, Functionalized metal–based nanoelectrocatalysts for water splitting, *Handbook of Functionalized Nanomaterials for Industrial Applications*, 1st edition, pp. 83–109, 2020, Elsevier.
DOI: [10.1016/B978-0-12-816787-8.00004-1](https://doi.org/10.1016/B978-0-12-816787-8.00004-1)
2. D. N. Karunaratne, G. K. Pamunuwa, I. H. V. Nicholas, Isuru R. Ariyaratna, Strategies for Enhancement of Bioavailability and Bioactivity of Curcumin, *Science of Spices and Culinary Herbs - Latest Laboratory, Pre-clinical, and Clinical Studies*, 1st edition, pp. 104–147, 2019, Bentham Science.
DOI: [10.2174/9781681087511119010007](https://doi.org/10.2174/9781681087511119010007)
1. D. N. Karunaratne, D. A. S. Siriwardhana, I. R. Ariyaratna, R. M. P. I. Rajakaruna, F. T. Banu, V. Karunaratne. Nutrient delivery through Nanoencapsulation, *Nutrient Delivery*, 1st edition, pp. 653–680, 2017, Elsevier.
DOI: [10.1016/B978-0-12-804304-2.00017-2](https://doi.org/10.1016/B978-0-12-804304-2.00017-2)

Research Articles in Preparation/Under Review

4. Isuru R. Ariyaratna and E. Miliordos, *Ab initio* investigation of the ground and excited states of TcO⁺ and RhO⁺: *In preparation.*
3. Isuru R. Ariyaratna and E. Miliordos, Electronic structure calculations of Mg(NH₃)⁺_{n=1–6} species: *In preparation.*

2. Isuru R. Ariyaratna and E. Miliordos, N₂ activation by frustrated Lewis pairs: Ground and excited state pathways: *In preparation*.
1. Isuru R. Ariyaratna and E. Miliordos, Ground and excited states of Ti(NH₃)₆^{0/+} Solvated electron precursors: *In preparation*.

Reviewing Activities in Journals

3. European Food Research and Technology.
2. Nanoscience & Technology: Open Access.
1. Recent Patents on Food, Nutrition & Agriculture.

Oral Presentations at Conferences

8. “Solvated electrons in metal bound crown–ethers: The case of M(12–Crown–4), M(15–Crown–5), and M(18–Crown–6) [M = Li, Na, K]”, This is Research Student Symposium at Auburn University, 2021.
7. “A superatomic perspective for metal–water clusters: The case of [Mg(H₂O)₆]^{0/+}”, 46th NOBCCChE Meeting at St. Louis, 2019.
6. “Aufbau Rules for Solvated Electron Precursors: The case of Li(NH₃)₄ and Na(NH₃)₄”, This is Research Student Symposium at Auburn University, 2019.
5. “Aufbau Rules for Solvated Electron Precursors: The case of Be(NH₃)₄^{0±}”, Sanibel Symposium at St. Simons island GA, 2019.
4. “Folate micro encapsulation using protein as a shell material”, Proceedings of the Peradeniya University International Research Sessions at Sri Lanka, 2014.
3. “Isolation and characterization of chickpea–protein and formation of CaCO₃ encapsulated protein microparticles”, Proceedings of the Peradeniya University International Research Sessions at Sri Lanka, 2014.
2. “Emulsion approach to develop an encapsulation method using nano CaCO₃ encased protein model”, Proceedings of the Postgraduate Institute of Science Research Congress at Sri Lanka, 2014.
1. “Curcumin microformulation towards solubility and delivery augmentation”, Driving Research Towards Economy: Opportunities and Challenges meeting at Sri Lanka, 2014.

Poster Presentations at Conferences

14. “Aufbau principle for diffuse electrons of double–shell metal ammonia complexes”, NOBCCChE Collaborative Conference, 2021.
13. “Electron solvation in metal–ammonia complexes”, ACS Spring Meeting, 2021. *Selected by the ACS PHYS division to present at live sessions.*
12. “Aufbau principle for diffuse electrons of double–shell metal ammonia complexes”, AIChE Meeting, 2020.
11. “Solvated electrons in metal bound crown–ethers: The case of M(12–Crown–4), M(15–Crown–5), and M(18–Crown–6) [M = Li, Na, K]”, 47th NOBCCChE Virtual Meeting, 2020.
10. “Extending the Aufbau principle of solvated electron precursors to the second solvation shell: The case of M(NH₃)₄@12NH₃ (M = Li, Be⁺, B²⁺)”, Southeastern Theoretical Chemistry Association Meeting at University of Tennessee, 2019.

9. "Story of the superatomic $\text{Mg}(\text{NH}_3)_{x=4,5,6}$ ", This is Research Student Symposium at Auburn University, 2019.
8. "CO activation by atomic Thorium: Ground and excited state reaction pathways", Sanibel Symposium at St. Simons island GA, 2019.
7. "Superatomic nature of $\text{Li}(\text{NH}_3)_4$ and $\text{Na}(\text{NH}_3)_4$ ", SERMACS at Augusta GA, 2018.
6. "Story of the super atomic $\text{Mg}(\text{NH}_3)_{x=4,5,6}$ ", SERMACS at Augusta GA, 2018.
5. "Aufbau Rules for Solvated electron precursors: The case of super atomic $\text{Mg}(\text{NH}_3)_4^{0,\pm}$ ", Southeastern Theoretical Chemistry Association Meeting at Louisiana State University, 2018.
4. "Electronic structures of $\text{Be}(\text{CO})_3$, $\text{Be}(\text{NH}_3)_3$, and $\text{Be}(\text{PH}_3)_3$ ", This is Research Student Symposium at Auburn University, 2018.
3. "Super atomic nature of $\text{Be}(\text{NH}_3)_4$ ", ACS Meeting at Louisiana, 2018.
2. "Oxygen unveils the versatile personality of beryllium: The case of $\text{BeO}_{n=1,2,4}$ ", This is Research Student Symposium at Auburn University, 2017.
1. "Oxygen unveils the versatile personality of beryllium: The case of $\text{BeO}_{n=1,2,4}$ ", Southeastern Theoretical Chemistry Association Meeting at University of Mississippi, 2017.

Oral Presentations at Auburn University

7. "First Principle Studies on Ground & Excited Electronic States: Chemical Bonding in Main-Group Molecules, Molecular Systems with Diffuse Electrons, and Water Activation using Transition Metal Monoxides", PhD Defense, Feb. 19, 2021.
6. "Electron Solvation and Super Atomic Nature of Metal-ligand Complexes" at COSAM Dean's research award ceremony, Apr. 16, 2019.
5. "Aufbau rules for solvated electron precursors" at COSAM Interdisciplinary colloquium, Feb. 5, 2019.
4. "Molecules Mimicking Atoms: Metal ammonia clusters" at Physical chemistry seminar, Oct. 2, 2018.
3. "Electron Solvation and Super Atomic Nature of Metal Ammonia Complexes" at Physical chemistry seminar, Mar. 6, 2018.
2. "Electronic structures of ground and excited states of MoO^+ , MoO^{2+} , MoO^- " at Physical chemistry seminar, Oct. 24, 2017.
1. "The versatile personality of Beryllium expressed in $\text{BeO}_{n=1,2,4}$ molecules" at Physical chemistry seminar, Mar. 7, 2017.

Teaching Experience

- 2015 – 2020 Teaching Assistant, Department of Chemistry and Biochemistry, Auburn University, AL, USA.
- 2015 Teaching Assistant, Department of Pharmacy, Faculty of Allied Health Science, University of Peradeniya, Sri Lanka.
- 2014 Teaching Assistant, Department of Chemistry, Faculty of Science, University of Peradeniya, Sri Lanka.

Expertise and Skills

- Computational programs: Molpro, Gaussian, QChem
- Visualization software: Avogadro, GaussView, IboView, VMD, GIMP, Origin
- vi editor

Additional Details

- Languages: English, Sinhala
- Professional memberships: ACS, AIChE, NOBCChE
- Number of citations: 222 (as of May 19, 2021)

References

- Prof. E. Miliordos: Auburn University, AL, 36849, USA (Email: ezm0048@auburn.edu).
- Prof. J. V. Ortiz: Auburn University, AL, 36849, USA (Email: jvo0001@auburn.edu).