

	Dr. Krishnamoorthy Arumugam
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Bio-Sketch (Optional) (Max: 200 words)

Dr. Krishnamoorthy Arumugam is an Associate professor at the Department of Chemistry, School of Engineering and Technology, Dhanalakshmi Srinivasan University, Trichy. He received his PhD in Theoretical Chemistry from the University of Manchester, United Kingdom. Successively, he worked as a Visiting Research Fellow at the School of Chemistry, University of Manchester, UK for seven months before moving to USA to take his Postdoctoral Research Fellow position. He spent two years at the Department of Earth and Environmental Sciences, University of Michigan, Ann Arbor, USA, with Prof. Udo Becker and explored computational actinide-mineral-water interface processes. Subsequently, he worked at the NIT/Trichy for one year as a Temporary Teaching Assistant and handled Engineering Chemistry-I and II for B.Tech. and Physical Chemistry (Theory and Practical) courses for M.Sc. Chemistry. Followed by this, he moved to SCANMAT Centre, Central University of Tamil Nadu (CUTN) as an NPDF and investigated actinide solid state chemistry. After the completion of the NPDF, he continued to work as a Visiting Scientist at the SCANMAT centre, CUTN, Thiruvavur for three years and extended his research horizon into computational materials chemistry.

Specialization

Computational Chemistry

Courses Offered

21CHY01	Engineering Chemistry
21CHYP1	Engineering Chemistry Laboratory
21NCP03	Environmental Science

Research Interests

- (1) Computational Actinide Chemistry
- (2) Computational Materials Chemistry
- (3) Computational Mineral-Water interface
- (4) Computational Catalysis

Awards/Honours/Affiliations

Outstanding Reviewer 2022 –Physical Chemistry Chemical Physics (RSC)
Overseas Research Studentship (2008-2011) (University of Manchester, UK).
M.Sc. Chemistry –Bharathidasan University Second Rank.
B.Sc. Chemistry –Gold Medallist.
B.Sc. Chemistry –Madurai Kamaraj University Fourth Rank.

Work History

Associate Professor, Dhanalakshmi Srinivasan University (Oct 2022 to till date).
Visiting Scientist, SCANMAT Centre, Central University of Tamil Nadu (Aug 2019 to Sep 2022).
National Post Doctoral Fellow (NPDF), SCANMAT Centre, Central University of Tamil Nadu (Aug 2017 to Aug 2019).

Temporary Teaching Assistant, National Institute of Technology, Trichy (Sep 2016 to June 2017).

Postdoctoral Research Fellow, University of Michigan, Ann Arbor, USA (Aug 2013 to July 2015).

Visiting Research Fellow, University of Manchester, United Kingdom.

Education History

Ph.D. Theoretical Chemistry (2012): University of Manchester, United Kingdom.

M.Sc. Chemistry (2008): School of Chemistry, Bharathidasan University, Trichy.

B.Sc. Chemistry (2006): APAC of Arts and Culture, Palani, affiliated to Madurai Kamaraj University.

Publications with link or DOI

1. "Investigation of ligand exchange reactions in aqueous uranyl carbonate complexes using computational approaches", Slimane Doudou, **Krishnamoorthy Arumugam**, David J. Vaughan, Francis R. Livens and Neil A. Burton., *Phys. Chem. Chem. Phys.*, **2011**, **13**, 11402-11411 (DOI: [10.1039/C1CP20617F](https://doi.org/10.1039/C1CP20617F)).

2. "Computational Redox Potential Predictions: Applications to Inorganic and Organic Aqueous Complexes, and Complexes Adsorbed to Mineral Surfaces", **Krishnamoorthy Arumugam** and Udo Becker, *Minerals* **2014**, **4**(2), 345-387 (DOI: [10.3390/min4020345](https://doi.org/10.3390/min4020345)).

3. "Density Functional Theory (DFT) Calculations of VI/V Reduction Potentials of Uranyl Coordination Complexes in Non-aqueous Solutions", **Krishnamoorthy Arumugam***, and Neil A. Burton, *Phys. Chem. Chem. Phys.*, **2019**, **21**, 3227-3241 (DOI: [10.1039/C8CP05412F](https://doi.org/10.1039/C8CP05412F)).

4. "The basis for reevaluating the reactivity of pyrite surfaces: spin states and crystal field d-orbital splitting energies of bulk, surface, edge, and corner Fe(II) ions", **Krishnamoorthy Arumugam***, Devon Renock, and Udo Becker, *Phys. Chem. Chem. Phys.*, **2019**, **21**, 6415-6431 (DOI: [10.1039/C8CP05459B](https://doi.org/10.1039/C8CP05459B)).

5. "Uranyl-bound tetra-dentate non-innocent ligands: Prediction of structure and redox behaviour using density functional theory", **Krishnamoorthy Arumugam*** and Neil A. Burton, *ChemPhysChem.*, **2019**, **20**, 1869-1878 (DOI: [10.1002/cphc.201900301](https://doi.org/10.1002/cphc.201900301)).

6. "NHC catalyzed green synthesis of functionalized chromones: DFT mechanistic insights and in vitro activities in cancer cells", Nithya Murugesu, Jebiti Haribabu, **Krishnamoorthy Arumugam**, Chandrasekar Balachandran, Rajagopal Swaathy, Anandaram Sreekanth, Ramasamy Karvembu, and Seenuvasan Vedachalam, *New Journal of Chemistry*, **2019**, **43**, 13509-13525 (DOI: [10.1039/C9NJ02650A](https://doi.org/10.1039/C9NJ02650A)).

7. "Disproportionation of the uranyl(V) coordination complexes in aqueous solution through an outer-sphere electron transfer", **Krishnamoorthy Arumugam*** and Neil A. Burton, *Inorg. Chem.* **2021**, **60**, **24**, 18832-18842 (DOI: [10.1021/acs.inorgchem.1c02575](https://doi.org/10.1021/acs.inorgchem.1c02575)).

8. "Actinyl adsorption and reduction on pyrite surface: insights from DFT calculations", **Krishnamoorthy Arumugam***, Sooyeon Kim, and Udo Becker, *ACS Earth and Space Chemistry*, **2022**, **6**, **3**, 571-581 (DOI: [10.1021/acsearthspacechem.1c00410](https://doi.org/10.1021/acsearthspacechem.1c00410)).

9. "X-ray Magnetic Circular Dichroism (XMCD) Spectra for Uranium Mono-Chalcogenides, UQ (Q=S, Se, and Te) from First Principles", **Krishnamoorthy Arumugam** and P. Ravindran, *Journal of Physical Chemistry C*, **2022**, **126**, **46**, 19792-19802 (DOI: [10.1021/acs.jpcc.2c05480](https://doi.org/10.1021/acs.jpcc.2c05480)).

Invited lectures

1. Given an invited lecture entitled, "*DFT modelling of Actinide-Mineral-Water Interface*", Krishnamoorthy Arumugam in the One day Indo-Norwegian Seminar, Department of Materials Science, SCANMAT Center, Central University of Tamil Nadu, Thiruvavur. September 28, 2017.
2. Given an invited lecture entitled, "*Bio-reduction of Actinides: Quantum Mechanical Explorations*", Krishnamoorthy Arumugam in the International Seminar on Frontiers in Biological Sciences, Departments of Biotechnology and Biochemistry, St. Joseph's College, Trichy. December 16, 2016.
3. Given an invited lecture entitled, "*Actinyl(VI/IV) Redox Potentials in Solution: Prediction and Assessment of DFT methods*", Krishnamoorthy Arumugam and Neil Burton, to the graduate students of computational mineralogy course, Department of Earth and Environmental Sciences, University of Michigan, Oct 28, 2013.

Oral and Poster Presentations

1. SERB-ACS online poster competition 2021. Presented a poster entitled, "*Ab initio first-principles modelling of actinide-chalcogenide solid state chemistry: Insights into electronic structure, bonding, magnetism, lattice dynamics, catalytic activity, and optical properties*", Krishnamoorthy Arumugam.
2. 248th ACS National Meeting and Exposition, At San Francisco, CA, USA. August 10-14, 2014. Given an oral presentation entitled, "*Electron transfer from Iron-sulfide redox-active mineral surfaces to actinyls: the role of interfacial water wires*", Krishnamoorthy Arumugam and Udo Becker.
3. Transformational Technologies in Molecular Simulations (Summer school). May 19-22, 2014 organized by the University of Wisconsin-Madison, Madison, USA. Presented a poster entitled, "*Actinyl adsorption into iron-sulfide mineral surfaces*", Krishnamoorthy Arumugam and Udo Becker.
4. MGMS Young Modellers' Forum meeting held on Nov 25, 2011 at London, UK. Presented a poster entitled, "*Actinyl reduction potentials in solution: An assessment of computational methods to achieve experimental accuracy*", Krishnamoorthy Arumugam, Neil A. Burton. Successfully obtained a travel bursary award.
5. Given an oral presentation entitled, "*DFT Investigation of Reduction Potentials of Uranyl Complexes in Solution*", School of Chemistry, the University of Manchester, July 7, 2011.
6. "The 2nd DTC Nuclear FiRST Winter School" at Barceló Palace Hotel, Buxton, UK, Jan 11-12, 2011 organised by the University of Manchester and University of Sheffield. Presented a poster entitled, "*Computational studies towards the stabilisation of U(V)*", Krishnamoorthy Arumugam, Neil A. Burton.
7. "The 1st DTC Nuclear FiRST Winter School" at Barceló Palace Hotel, Buxton, UK, Jan 12-14, 2010 organised by the University of Manchester and University of Sheffield. Presented a poster entitled, "*Modelling Actinide Chemistry in Solution and at Mineral Surfaces*", Krishnamoorthy Arumugam, Slimane Doudou, Neil A. Burton.