

DrS.ANGELINE VEDHA

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Web:

M.Sc	Chemistry	The American College	1999
B.Sc	Chemistry	Lady Doak College, Madurai	1997

Ph.D. Details**Title of Thesis**

On the oxidized state and Inhibition of [NiFeSe]
Hydrogenase and concurrent binding of [NiFe]

Area of Specialization

Computational Chemistry

Research Supervisor

Prof. P. Venuvanalingam

Research Centre

Bharathidasan University

Year of Award

2015

Cleared NET / SET :

NET

Details**Year of Passing**

2000

Additional Qualification**Name of Course**

NA

Place of Study**Date****Duration****Work Experience****Name of Institution**

Bishop Heber College

Address of Institution

Bishop Heber College
Trichy

Designation

Associate Professor

From

18-01-2000

To

31-3-2035

Teaching / Research Experience

U.G. : 17 years

P.G. : 17 years

M.Phil. -

Ph.D. -

Research Guidance

U.G. :

P.G. : 17 years

M.Phil. :

Ph.D. :

Field Experience

Type	Name of the Sector	Designation	From	To
	NA			

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1.	Conferences / workshops / Seminars Attended	7
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3.	Publication in Journals	13
4.	Publication in Books	0
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6.	Conferences / Workshops / Seminars Organised	5
7.	Research Projects	0
8.	Resource Person	3
9.	Consultancy	0
10.	Awards Recieved	1
11.	Patent	0
12.	Extension Activities Undertaken	0
13.	Professional Membership	1
14.	M.Phil. / Ph.D. Produced	0 / 0

1. National level Workshop on **"Research Based Pedagogical Tools for STEM teacher Trainers"** sponsored by Department of Biotechnology (DBT), Government of India, and Newton Bhabha Fund of the British Council organized by Indian Institute of Chemical Technology at New Delhi during 06/12/2017 to 09/12/2017.
2. National level Workshop on **"Research Based Pedagogical Tools for STEM teachers"** sponsored by Department of Biotechnology (DBT), Government of India, and Newton Bhabha Fund of the British Council organized by Centre of Excellence in Science and Mathematics Education (COESME), Indian Institute of Science Education (IISER) Pune at Kochi during 11/10/2017 to 14/10/2017.
3. National level Workshop on **"Gaussian Workshop"** sponsored by Gaussian Inc, and CLRI, Chennai and IIT Chennai organized by Gaussian Inc, and CLRI, Chennai and IIT Chennai at IIT during 07/12/2012 to 12/12/2012.
4. -1 level Conference on **"International Conference on Applied Theory on Molecular Systems in November 2011 conducted by the IICTE, Hyderabad"** sponsored by Indian Institute of Chemical Technology organized by Indian Institute of Chemical Technology at Hyderabad during 09/11/2011 to 13/11/2011.
5. International level Workshop on **"Understanding Molecular Simulations"** sponsored by CSIR organized by Jawaharlal nehru Centre for Advanced Scientific research at Bengaluru during 17/08/2009 to 28/08/2009.

Research Papers Presented

- 2

1. **"Hypercoordinated bonds in (Si₆X₁₄)₂-"** in the International conference on *International Conference on Applied Theory on Molecular Systems in* sponsored by , organized by IICTE, Hyderabad at Hyderabad during 11/11/2011 to 01/01/1900.
2. **"An QTAIM investigation of the hypervalent Si"** in the International conference on *international conference on Inorganic Materials* sponsored by DBT, organized by Bharathidasan University at Trichy during 01/01/1900 to 01/01/1900.



1. **"Enhanced luminescence efficiency of structurally tailored new coumarin-based heterocyclic organic materials: a DFT/TD-DFT study"** published in Theoretical Chemistry Accounts (PEER REVIEW) Vol. 138, Issue No. 4, April 2019 ISSN : ---.
2. **"DFT-TDDFT framework of diphenylamine based mixed valence compounds for optoelectronic applications–Structural modification of p-acceptors"** published in Computational Materials Science (PEER REVIEW) Vol. 162, Issue No. , February 2019 ISSN : 0927-0256.
3. **"A new turn in codon–anticodon selection through halogen bonds"** published in Physical Chemistry Chemical Physics (PEER REVIEW) Vol. 16, Issue No. 16, January 2017 ISSN : 1463-9084.
4. **"Noncovalent interactions between the second coordination sphere and the active site of [NiFeSe] hydrogenase"** published in RSC Advances (PEER REVIEW) Vol. 6, Issue No. 85, August 2016 ISSN : 2046-2069.
5. **"Insights from the computational studies on the oxidized as-isolated state of [NiFeSe] hydrogenase from D. vulgaris Hildenborough"** published in Physical Chemistry Chemical Physics (PEER REVIEW) Vol. 17, Issue No. 32, July 2015 ISSN : 1463-9084.
6. **"Computational evaluation of optoelectronic and photophysical properties of unsymmetrical distyrylbiphenyls"** published in RSC Advances (PEER REVIEW) Vol. 4, Issue No. 95, October 2014 ISSN : ---.
7. **"The nature of hydrogen bonding in R22(8) crystal motifs – a computational exploration"** published in Molecular Physics (PEER REVIEW) Vol. 112, Issue No. , July 2014 ISSN : 0026-8976.
8. **"Atomic partitioning of M–H₂ bonds in [NiFe] hydrogenase – a test case of concurrent binding"** published in Physical Chemistry Chemical Physics (PEER REVIEW) Vol. 16, Issue No. 22, April 2014 ISSN : 1463-9084.
9. **"The metal delivery mechanism of transferrin and the role of bent metallocene metals towards anticancer activity – a theoretical exploration"** published in RSC Advances (PEER REVIEW) Vol. 4, Issue No. 19, December 2013 ISSN : 2046-2069.
10. **"A DFT/TDDFT modelling of bithiophene azo chromophores for optoelectronic applications"** published in Dyes and Pigments (PEER REVIEW) Vol. 100, Issue No. , September 2013 ISSN : 1873-3743.
11. **"On the Nature of Hypercoordination in Dihalogenated Perhalocyclohexasilanes"** published in Journal of Physical Chemistry A (PEER REVIEW) Vol. 117, Issue No. 16, March 2013 ISSN : 1089-5639.

12. **"Designing benzosiloles for better optoelectronic properties using DFT & TDDFT approaches"** published in Physical Chemistry Chemical Physics (PEER REVIEW) Vol. 14, Issue No. 41, July 2012 ISSN : 1463-9084.
13. **"Tuning Nonlinear Optical and Optoelectronic Properties of Vinyl Coupled Triazene Chromophores: A Density Functional Theory and Time-Dependent Density Functional Theory Investigation"** published in Journal of Physical Chemistry A (PEER REVIEW) Vol. 116, Issue No. 18, April 2012 ISSN : 1089-5639.

Conferences / Workshops / Seminars Organised

- 5

1. International level Conference Entitled **"Chemical Research and Innovations Today"** at Bishop Heber College, sponsored by UGC, during 22/01/2020 to 22/01/2020.
2. International level Conference Entitled **"Applications of Basic Sciences"** at Bishop Heber college, Tiruchirappalli-620 017, sponsored by , during 19/11/2019 to 21/11/2019.
3. College level Conference Entitled **"Young Investigators Meet"** at Bishop Heber College, sponsored by DBT - Star Scheme, during 28/02/2019 to 28/02/2019.
4. International level Conference Entitled **"Chemistry for Renewable Energy"** at Bishop Heber college, Tiruchirappalli-620 017, sponsored by , during 25/02/2016 to 26/02/2016.
5. International level Conference Entitled **"Chemistry in Synergy with materials and Biology"** at Bishop Heber college, Tiruchirappalli-620 017, sponsored by , during 10/01/2014 to 11/01/2014.

Awards Recieved

- 1

Award Name	Presented by	Year	Level	Instituted by / Place	amount
NA		01/01/1900	SELECT		

PROFESSIONAL MEMBERSHIP

- 1

- * Member of Board of Studies of Sri Saradha College Salem during 01/01/2019 - Till Date

TRAINING PROGRAMME

- 1

- # NATIONAL level Training by MHRD IISER & Newon Bhabha fund on **"Research Based Pedagogical Tools Level 2"** Sponsored by MHRD IISER & Newon Bhabha fund, Organized by IISER PUNE at INSA New Delhi during 06/12/2017 - 09/12/2017.

1. College level Invited Lectures on **"Noncovalent interactions and QTAIM in the Winter School on Computational Modelling"** at Holy Cross College, Tiruchirappalli- 620 008, 27/02/2020.
2. College level Seminar on **"Rev Fr Moollel Endowment Lecture"** at St Josephs College Trichy, 05/02/2019.
3. State level Seminar on **"Current Trends in Chemistry"** at The American College Madurai, 24/09/2018.



Signature of Staff
(S.ANGELINE VEDHA)