

Curriculum Vitae of Dr. N. Arul Murugan

Current position : Researcher (Forskare)
: Department of Theoretical Chemistry
: School of Biotechnology
: Royal Institute of Technology
: Stockholm, Sweden

Education:

- **Ph.D**, 2005, Computational Chemistry, SSCU, Indian Institute of Science, Bangalore.
(**Thesis title: Molecular simulations of temperature induced disorder and pressure induced ordering in organic molecular crystals. Thesis supervisor: Prof. S. Yashonath**)
- **M.Sc**, 1998, Chemistry, GRI-Deemed University, Dindigul.
(**Thesis title: Phytochemical reinvestigation and pharmacological studies of the roots of Dalbergia Sissoides (GRAH). Thesis supervisor: Prof. N.S. Nagarajan**)
- **B.Sc**, 1996, Chemistry, Physics, Maths, R.D.M. Govt. Arts college, Sivaganga.

Academic experience:

- Researcher, Department of Theoretical Chemistry, School of Biotechnology, Royal Institute of Technology (KTH), Stockholm, Sweden.
- Postdoctoral fellow, Department of Theoretical Chemistry, School of Biotechnology, Royal Institute of Technology (KTH), Stockholm, Sweden (with **Prof. Hans Ågren**).
- Postdoctoral fellow, Department of Physics and Nuclear Engineering, Polytechnical University of Catalunya (UPC), Barcelona, Spain (with **Prof. J.Ll. Tamarit**).
- Postdoctoral fellow, Department of Theoretical Chemistry, School of Biotechnology, KTH, Stockholm, Sweden (with **Prof. Hans Ågren and Dr. Håkan Hugosson**).
- Postdoctoral fellow, Laboratory for Physics of Polymers, Universite Libre de Bruxelles (ULB), Brussels, Belgium (with **Prof. J.-P. Ryckaert**).
- R&D assistant and Postdoctoral fellow, Condensed Matter Theory Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India (with **Prof. S. Yashonath**).

Fellowships, awards and recognition:

- Juan de la Cierva postdoctoral fellowship (JDLC grant funded by Spanish Ministry of Science and Innovation)
- Wenner-Gren postdoctoral fellowship
- FNRS Postdoctoral fellowship (funded by Belgian National Fund for scientific research)
- Biography selected for *Marquis who's who in the world*, 2010 Edition
- Reviewer for Journal of Physical Chemistry, Physical Chemistry Chemical Physics, Spectrochimica Acta, South african journal of chemistry
- Qualified joint CSIR-UGC JRF/Eligibility for lectureship and Graduate Aptitude Test in Engineering (GATE)
- Qualified National Merit Scholarship (Class X)

Publications list:

[1] **N. Arul Murugan***, P.C. Jha, S. Yashonath and S. Ramasesha,
High Pressure phase of biphenyl in room temperature: A Monte Carlo study.
J. Phys. Chem. B., **108**, 4178(2004).

[2] **N. Arul Murugan** and S. Yashonath*,
Structure, energetics and dynamics of pedal-like motion in stilbene from molecular simulation and ab initio calculations.
J. Phys. Chem. B., **108**, 17403(2004).

[3] **N. Arul Murugan** and S. Yashonath*,
Pressure Induced Ordering Transition in Adamantane : A Monte Carlo Simulation Study.
J. Phys. Chem. B., **109**, 2014(2005).

[4] **N. Arul Murugan** and S. Yashonath*,
Pressure induced orientational ordering in p-terphenyl.
J. Phys. Chem. B., **109**, 1433(2005).

[5] **N. Arul Murugan** and S. Yashonath*,
Effect of pressure on pedal motion in stilbene molecular crystals and its dependence on crystallographic site.
J. Phys. Chem. B., **109**, 12107(2005).

[6] **N. Arul Murugan**, S. Yashonath*, R.S.Rao, S. Ramasesha and B.K.Godwal,
High pressure study of adamantane: variable shape simulations up to 26 GPa.
J. Phys. Chem. B., **109**, 17296(2005).

[7] **N. Arul Murugan***,
Orientational melting and reorientational motion in cubane molecular crystal: a molecular simulation study.
J. Phys. Chem. B., **109**, 23955(2005).

- [8] N. Arul Murugan*,
Temperature induced dynamical conformational disorder in 4-vinyl benzoic acid molecular crystals: A Monte Carlo simulation study.
J. Chem. Phys., **123**, 094508(2005).
- [9] N. Arul Murugan*,
What does pressure decide to cook with orientationally disordered plastic phase of cubane molecular crystal: an orientational glass or crystal?
J. Chem. Phys., **123**, 244514(2005).
- [10] N. Arul Murugan* and Håkan Hugosson,
Investigations into conformational transitions and solvation structure of a 7-piperidino-5,9-methanobenzo[8] annulene in water.
Phys. Chem. Chem. Phys., **40**, 6135(2008).
- [11] N. Arul Murugan*, Håkan Hugosson and Hans Ågren,
Solvent Dependence on Conformational Transition, Dipole Moment, and Molecular Geometry of 1,2-Dichloroethane: Insight from Car-Parrinello Molecular Dynamics Calculations.
J. Phys. Chem. B. (Letter), **112**, 14673(2008).
- [12] K. J. de Almeida, N. Arul Murugan*, Z. Rinkevicius, Håkan Hugosson, Olav Vahtras, Hans Ågren and Amary Cesar,
Conformations, structural transitions and visible near-infrared absorption spectra of four-, five- and six-coordinated Cu(II) aqua complexes.
Phys. Chem. Chem. Phys., **3**, 508(2009).
- [13] N. Arul Murugan* and Håkan Hugosson,
Solvent Dependence of Conformational Distribution, Molecular Geometry, and Electronic Structure in Adenosine.
J. Phys. Chem. B., **113**, 1012(2009).
- [14] N. Arul Murugan* and Hans Ågren,
Role of Dynamic Flexibility in Computing Solvatochromic Properties of Dye-Solvent Systems: o-Betaine in Water.
J. Phys. Chem. A., **113**, 2572(2009).
- [15] N. Arul Murugan* and Hans Ågren,
1,2-Dichloroethane in Haloalkane Dehalogenase Protein and in Water Solvent: A Case Study of the Confinement Effect on Structural and Dynamical Properties.
J. Phys. Chem. B. (Letter), **113**, 3257(2009).
- [16] N. Arul Murugan*, Z. Rinkevicius and Hans Ågren,
Solvent Dependence on Bond Length Alternation and Charge Distribution in Phenol Blue: A Car-Parrinello Molecular Dynamics Investigation.
J. Phys. Chem. A. (Letter), **113**, 4833(2009).
- [17] N. Arul Murugan* and P.C. Jha,

Pressure dependence of crystal structure and molecular packing in anthracene.
Molecular Physics, **107**, 1689(2009).

[18] **N. Arul Murugan***, P.C. Jha and Hans Ågren
Solvation shell structure of cyclooctylpyranone in water solvent and its comparative structure, dynamics and dipole moment in HIV Protease.
Phys. Chem. Chem. Phys., **3**, 508(2009).

(This article has been selected for **Highlights in Chemical Biology: Research Articles, issue 9, 2009**)

[19] **N. Arul Murugan*** and A. Sayeed,
Thermal behavior of disordered phase of caffeine molecular crystal: A variable shape Monte Carlo simulation study.
J. Chem. Phys., **130**, 204514(2009).

[20] M. Rovira-Esteva*, **N. Arul Murugan**, L.C. Pardo, S. Busch, M.D. Ruiz-Martin, M.-S. Appavou, J.Ll. Tamarit, C. Smuda, T. Unruh, F.J. Bermejo, G.J. Cuello, and S.J. Rzoska
Microscopic structures and dynamics of high- and low-density liquid trans-1,2-dichloroethylene.
Phys. Rev. B. (Brief reports), **81**, 092202(2010).

[21] **N. Arul Murugan***, P.C. Jha, Z. Rinkevicius, Kenneth Ruud and Hans Ågren
Modeling of solvatochromism of phenol blue in water using hybrid-QM/MM and Zindo calculation.
J. Chem. Phys., **132**, 234508(2010). (This article has been selected for **Virtual Journal of Biological Physics Research, Volume 20, Issue 1, July 1, 2010**)

[22] **N. Arul Murugan**, Jacob Kongsted, Z. Rinkevicius and Hans Ågren*
Break-down of the "first hyperpolarizability/ bond-length alternation parameter" relationship.
Proc. Natl. Acad. Sci. (USA), **107 (38)** 16453(2010).

[23] **N. Arul Murugan***, J. Kongsted, Z. Rinkevicius, K. Aidas and Hans Ågren
Modeling the structure and absorption spectra of stilbazolium merocyanine in polar and nonpolar solvents using hybrid QM/MM techniques.
J. Phys. Chem. B, **114(32)**, 13349(2010).

[24] **N. Arul Murugan***, Z. Rinkevicius and Hans Ågren
Modeling of solvatochromism of Nile red in water.
International Journal of Quantum Chemistry, **111**, 1521(2011).

[25] **N. Arul Murugan***, J. Kongsted, Z. Rinkevicius and Hans Ågren
Demystifying the solvatochromic reversal in Brooker's merocyanine dye
Phys. Chem. Chem. Phys. (Communications), **13**, 1290(2011).

[26] **N. Arul Murugan***,
Modeling solvatochromism of a quinolinium betaine dye in water solvent using sequential hybrid QM/MM and semicontinuum approach.
J. Phys. Chem. B, **115**, 1056(2011).

- [27] **N. Arul Murugan***, S. Chakrabarti and Hans Ågren
Solvent Dependence of Structure, Charge Distribution and Absorption Spectrum in the Photochromic Merocyanine-Spiropyran Pair
J. Phys. Chem. B, **115**, 4925(2011).
- [28] Z. Rinkevicius*, **N. Arul Murugan**, J. Kongsted, A. Steindal, K. Aidas and Hans Ågren
A density functional theory/molecular mechanics approach for electronic g-tensors of solvated molecules
J. Phys. Chem. B, **115**, 4350(2011).
- [29] **N. Arul Murugan***, J. Kongsted, Z. Rinkevicius, K. Aidas, K.V. Mikkelsen and Hans Ågren
Hybrid density functional theory / molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution
Phys. Chem. Chem. Phys., **12506**, 13(2011).
- [30] M. Rovira-Esteva*, **N. Arul Murugan**, L.C. Pardo, S. Busch, J.Ll. Tamarit, G.J. Cuello, and F.J. Bermejo
Interplay of intramolecular and intermolecular structure of 1,1,2,2-tetrachloro-1,2-difluoroethane.
Phys. Rev. B, **84**, 064202(2011).
- [31] Z. Rinkevicius*, **N. Arul Murugan**, J. Kongsted, B. Frecus, A. Steindal, and Hans Ågren
Density functional restricted-unrestricted/molecular mechanics theory for hyperfine coupling constants of molecules in solution
J. Chem. Theory Comput., **7**, 3261(2011).
- [32] **N. Arul Murugan***, J. Kongsted, Z. Rinkevicius, and Hans Ågren
Color modeling of protein optical probes
Phys. Chem. Chem. Phys.(Communication), **14**, 1107(2012) (DOI: 10.1039/C1CP23060C).
- [33] Z. Rinkevicius*, B. Frecus, **N. Arul Murugan**, J. Kongsted, O. Vahtras, and Hans Ågren
Encapsulation influence on EPR parameters of spin-labels: 2,2,6,6-tetramethyl-4-methoxypiperidine-1-oxyl in cucurbit[8]uril
J. Chem. Theory Comput., **8**, 257(2012).
- [34] S. Selvaraj, **N. Arul Murugan***, Hans Ågren
 $A\beta^+$ induced planarization, conformational arrest and metallochromic shift in a pyrimidine dione dye: Insight from integrated hybrid quantum-classical calculations
Phys. Chem. Chem. Phys., **14(7)**, 2339(2012).
- [35] Muriel Rovira-Esteva, **N. Arul Murugan**, L.C. Pardo, S. Busch, J. Tamarit, G. J. Cuello and F.J. Bermejo
Differences in first neighbor orientation behind the anomalies in the low and high density trans-

1,2-dichloroethene liquid

J. Chem. Phys., **00**, 000(2012).

[36] N. Arul Murugan*, K. Aidas, J. Kongsted, Z. Rinkevicius, and Hans Ågren
NMR spin-spin coupling constants in polymethine dyes as polarity indicators
Chemistry: A European Journal, **00**, 0000(2012).

* published as corresponding author

Conferences attended:

- 2011 “MONAMI-Meeting”, Indian Institute of Science, Bangalore, India.
- 2010 “Scalalife Kickoff meeting”, PDC, KTH, Stockholm, Sweden.
- 2010 “Nordic-China symposium on molecular Bio- and Nanoscience”, University of Science and Technology of China, Hefei, China.
- 2009 “MONAMI-Meeting”, MPI, Stuttgart, Germany.
- 2008 “Computational Chemistry Autumn Meeting 2008”, Kongsvinger, Norway.
- 2008 “Correspondence between Concepts in Chemistry and Quantum Chemistry”, Valadalen, Sweden.
- 2008 Wenner-Gren Foundations International Symposium “Theoretical Biochemistry - Methods and Applications”, Stockholm, Sweden.
- 2005 “International Conference on Statistical Mechanics of Plasticity and Related Stabilities”, Materials Research Center, Indian Institute of Science, Bangalore, India.
- 2004 “DAE-BRNS Symposium on Theoretical Chemistry”, Bhaba Atomic Research Center, Mumbai, India.
- 2003 “Practicals of Parallel Computing in the Physical Sciences”, Indian Institute of Science, Bangalore, India.
- 2001 “Computational Techniques for Condensed Matter”, Indian Institute of Science, Bangalore, India.
- 2001 “International Symposium on Solid State and Materials Chemistry”, Indian Institute of Science, Bangalore, India.
- 2000 “Structure and Dynamics of Complex Chemical Systems”, Indian Institute of Science, Bangalore, India.

Research Interests:

- Car-Parrinello mixed quantum mechanics-molecular mechanics simulations (CPMD-QM/MM) of organic, biological molecules, proteins and metalloproteins in aqueous and non-aqueous solvents.
- Modeling of solvatochromism, thermochromism, enzymochromism and metallochromism.
- *Ab initio* electronic structure calculations based materials design.
- Molecular simulation investigations of structure and dynamics of complex systems such as hydrogen bonding network liquids, polymers, proteins and other biomolecules.
- Absorption spectra, hyperpolarizability, two photon absorption, EPR and NMR spectra calculation for organic molecules, inorganic complexes and metalloproteins.
- Structural transformations, orientational and conformational disorder and polymorphism in organic molecular solids and liquid-liquid transition.
- Structure and dynamics of materials at extreme pressure and temperature.

Coding skills and experience in using softwares:

- Involved in the development of Monte Carlo, molecular dynamics codes for atomic, molecular and polymeric systems.
- Experience in performing CPMD-QM/MM calculations for metalloproteins, proteins and organic molecules in solvents.
- Experience in using Gaussian98/03/09 and Dalton2.0 (*ab initio* electronic structure calculation packages).
- Experience in using Amber8 and DL_POLY to perform molecular dynamics calculations.
- Experience with CSD (Cambridge Structure Database for small molecules) and protein database.

Computational background:

- **Programming Languages and scripting skills:**
Fortran77/90, C/C++, parallel programming using MPI (Message passing interface library), matlab, web design using HTML/Perl.

Personal details:

Date of birth : 12.03.1976
Place of birth : Paramakudi, Ramnad, India
Nationality : Indian
Marital status : Married
E-mail : murugan@theochem.kth.se, arul.murugan.at.kth@gmail.com
Phone : 0046 855378418 (Office)
0046 768961432