SALAI CHEETTU AMMAL

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EDUCATION

Bharathidasan University Tiruchirappalli, India

Ph. D. in Chemistry, October 1998
Thesis: "Origin and nature of lithium and hydrogen bonding interactions in complexes of LiF/HF with various bases: An ab initio molecular orbital study"
Advisor: Professor P. Venuvanalingam Grade: "Highly commended"

M.Sc in Chemistry, May 1992 (Master's degree)
Thesis: "Quantum and molecular mechanical studies on conformations of methoxylamines"
Advisor: Professor P. Venuvanalingam Grade: "First class"

Madurai Kamaraj University Madurai, India
B.Sc in Chemistry, May 1990 (undergraduate degree)

Indian Institute of Science Bangalore, India
Visiting scholar in the Solid State & Structural Chemistry Unit, April – June 1993, April – June 1994, April – June 1995
- Conducted collaborative research on Ph.D. thesis under Professor M. S. Hegde.

National Chemical Laboratory Pune, India
Visiting scholar in the Physical and Material Chemistry division, April – May 1996
- Conducted collaborative research on Ph.D. thesis under Professor Sourav Pal.

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PROFESSIONAL EXPERIENCE

University of South Carolina Columbia Campus, South Carolina
Department of Chemical Engineering
Research Assistant Professor *Oct. 16, 2013 – present*
Research areas: Computational catalysis – Rational (nano)material design – Interface Catalysis – Electrocatalysis- Multiscale modeling
- Heterogeneous catalysis at metal-oxide interface relevant to energy conversion and chemical production.
- Multiscale modeling of anode reactions in solid oxide fuel cells ranging from industrial catalysts to novel perovskite materials.

University of South Carolina Columbia Campus, South Carolina
Department of Chemical Engineering
Postdoctoral Associate with Dr. Andreas Heyden *March 1, 2008 – Oct. 15, 2013*
Research areas: Computational catalysis – Rational (nano)material design – Multiscale modeling

- Investigated the effect of catalyst support on the structure, surface composition, and catalytic activity of oxide supported metal clusters and nanoparticles.
- Investigated the mechanism of fuel electro-oxidation reactions at the Ni/YSZ anode interface and a novel perovskite anode surface.

Rikkyo University Tokyo, Japan
Department of Chemistry
Postdoctoral Researcher with Prof. Hiroshi Yamataka *April 1, 2004 – June 30, 2005*
- Investigated the kinetic selectivity of mechanistically borderline reactions such as Beckmann rearrangement reaction and isomerization of benzylideneanilines using ab initio molecular dynamics simulations.

The University of Tokyo Tokyo, Japan
Department of Chemistry
Postdoctoral Researcher with Prof. Eiichi Nakamura *April 1, 2003 – March 31, 2004*
- Investigated homogeneous catalysis by polynuclear transition metal complexes using density functional theory – gained insights on the promotional effect of the second metal in the catalytic activity of a thiolate-bridged diruthenium complex in nucleophilic substitution reactions of propargylic alcohols.
- Identified a new type of L-shaped three-center two-electron bonding produced by acetylene/carbenium ion interaction.

Osaka University Osaka, Japan
Institute of Scientific and Industrial Research
JSPS Postdoctoral Fellow with Prof. Hiroshi Yamataka *March 1, 2001–February 28, 2003*
- Uncovered the effects of dynamics on the intramolecular rearrangement of protonated pinacolyl alcohol - chemical reactions may in fact proceed through a reaction route totally different from the intrinsic reaction coordinate (IRC) route and its concomitant products on the potential energy surface (recognized for publication in "Science")
- Performed ab initio and DFT calculations on the acid-catalyzed ionization of neophyl and phenylethyl alcohols to investigate whether a variation of the transition state structure is reflected in the kinetic isotope effects and linear free energy relationship.

Institute for Molecular Science Okazaki, Japan
Theoretical Division I
Postdoctoral Fellow with Prof. Suehiro Iwata *October 15, 1999 – March 31, 2000*
- Calculated the weakly bound reactant and product complexes in the hydrogen abstraction reactions of an OH radical with hydrocarbons – radical reactions that are important in the current atmospheric environmental issue.

Tohoku University Osaka, Japan
Department of Material Science
Postdoctoral Fellow with Prof. Akira Miyamoto *April 1, 1998 – March 31, 1999*
- Studied the surface structure and polarity of ZnO and its band gap modulation by doping with various metals.
- Investigated the adsorption of various molecules on Ru cluster and V_2O_5 (010) surface.

Bharathidasan University Tiruchirappalli, India
Department of Chemistry
Ph.D. student researcher with Prof. P. Venuvanalingam *September 1, 1992–March 31, 1998*

- Identified the nature of lithium and hydrogen bonding interactions at orbital level in complexes of LiF/HF with various bases – gained significant insights into the origin of lithium bonds with different donors which influences greatly the geometry and strength of the complexes.
- Investigated the donor-acceptor interactions of halogens with n- and π-donors using ab initio calculations together with ultraviolet photoelectron spectroscopy and electron energy loss spectroscopy measurements.

Master's student researcher with Prof. P. Venuvanalingam *July 1, 1991 – April 30, 1992*

- Performed conformational analysis of methoxylamines using molecular mechanics and semi-empirical methods.

PROFESSIONAL ACTIVITIES/AWARDS

- 2005-present: Manuscript reviewer for Organic Letters, Journal of Physical Chemistry, and RSC Advances
- *JSPS Postdoctoral Research Fellowship,* 2001 – 2003
- *Japan Science and Technology (JST) Postdoctoral Research Scholarship,* 2000, 1998-1999
- *National Predoctoral Research Fellowship and Lectureship by University Grants Commission (UGC), India,* 1993-1998
- Session chair at the 'International Conference on Solid State Devices and Materials (1998)', held in Hiroshima, Japan
- Outstanding presentation award at the 'International Conference on Molecular Association', Aligarh Muslim University, Aligarh (India): March 18-20, 1996.

TEACHING EXPERIENCE

University of South Carolina Columbia, South Carolina
Postdoctoral Researcher and Research Assistant Professor

- Providing guidance to graduate students, 2008 – current

Bharathidasan University Tiruchirappalli, India
Ph.D. Student

- Provided guidance to Master's students, 1996 – 1998
- Taught quantum chemistry classes occasionally in Graduate classes

PUBLICATIONS

Series:

[1] Ammal, S. C. and Yamataka, H., How Does Carbocation Stability Control the Beckmann Rearrangement Reaction?, Recent Developments in Carbocation and Onium Ion Chemistry. Laali, K. Ed.; ACS Symposium series **965**; American Chemical Society: Washington, DC, **2007**; Chapter 17.

Journals:

[48] Ammal, S. C., Heyden, A., Water-Gas Shift Catalysis at Corner Atoms of Pt Clusters in Contact with a TiO_2 (110) Support Surface, *ACS Catalysis* **2014**, 4, 3654-3662.

[47] Suthirakun, S., Ammal, S. C., Munoz-Garcia, A. B., Xiao, G., Chen, F., zur Loye, H.-C., Carter, E. A., Heyden, A., Theoretical Investigation of H_2 Oxidation on the $Sr_2Fe_{1.5}Mo_{0.5}O_6$ (001) Perovskite Surface under Anodic Solid Oxide Fuel Cell Conditions, *Journal of American Chemical Society* **2014**, 136, 8374-8386.

[46] Aranifard, S., Ammal, S. C., Heyden, A., On the importance of the associative carboxyl mechanism for the water-gas shift reaction at Pt/CeO_2 interface sites, *Journal of Physical Chemistry C* **2014**, 118, 6314-6323.

[45] Aranifard, S., Ammal, S. C., Heyden, A., On the Importance of Platinum-Ceria Interfaces for the Water-Gas Shift Reaction. *Journal of Catalysis* **2014**, 309, 314-324.

[44] Suthirakun, S., Xiao, G., Ammal, S. C., F. Chen, H.-C. zur Loye, Heyden, A., Rational Design of Mixed Ionic and Electronic Conducting Perovskite Oxides for Solid Oxide Fuel Cell Anode Materials: A Case Study for Doped $SrTiO_3$. *Journal of Power Sources* **2013**, 245, 875-885.

[43] Ammal, S. C., Heyden, A., Origin of the Unique Activity of Pt/TiO_2 Catalysts for the Water-Gas Shift Reaction. *Journal of Catalysis* **2013**, 306, 78-90.

[42] Galhenage, P., Ammal, S. C., Yan, H., Duke, A. S., Tenney, S. A., Heyden, A., Chen, D. A., Nucleation, Growth and Adsorbate-induced Changes in Composition for Co-Au Bimetallic Clusters on TiO_2. *Journal of Physical Chemistry C* **2012**, 116, 24616-24629.

[41] Suthirakun, S., Ammal, S. C., Xiao, G., Chen, F., Huang, K., zur Loye, H.-C., Heyden, A., Obtaining mixed ionic/electronic conductivity in perovskite oxides in a reducing environment: A computational prediction for doped $SrTiO_3$. *Solid State Ionics* **2012**, 228, 37-45.

[40] Ammal, S. C., Heyden, A., Combined DFT and Microkinetic Modeling Study of Hydrogen Oxidation at the Ni/YSZ Anode of Solid Oxide Fuel Cells. *Journal of Physical Chemistry Letters* **2012**, 3, 2767-2772.

[39] Aranifard, S., Ammal, S. C., Heyden, A., Nature of Pt_n/CeO_2 (111) interface under water-gas shift reaction conditions: A constrained ab initio thermodynamics study. *Journal of Physical Chemistry C* **2012**, 116, 9029-9042.

[38] Suthirakun, S., Ammal, S. C., Xiao, G., Chen, F., zur Loye, H.-C., Heyden, A., Density functional theory study on the electronic structure of n- and p-type doped $SrTiO_3$ at anodic solid oxide fuel cell conditions. *Physical Review B* **2011**, 84, 205102.

[37] Ammal, S. C., Heyden, A., Nature of Pt_n/TiO_2 (110) interface under Water-Gas Shift reaction conditions: A constrained ab initio thermodynamics study. *Journal of Physical Chemistry C* **2011**, 115, 19246-19359.

[36] Tenney, S. A., Ratliff, J. S., Roberts, C. C., He, W., Ammal, S. C., Heyden, A., Chen, D. A., Adsorbate-Induced Changes in the Surface Composition of Bimetallic Clusters: Pt-Au on TiO_2 (110). *Journal of Physical Chemistry C* **2010**, 114, 21652-21663.

[35] Ammal, S. C., Heyden, A., Modeling the noble metal/TiO_2 (110) interface with hybrid DFT functionals: A periodic electrostatic embedded cluster model study. *Journal of Chemical Physics* **2010**, 133, 164703.

[34] Yamataka, H., Sato, M., Hasegawas, H., and Ammal, S. C., Dynamic Path Bifurcation for the Beckmann Reaction: Observation and Implication. *Faraday Discussion* **2010,** 145, 327.

[33] Basheer, A., Yamataka, H., Ammal, S. C., and Rappaport, Z., Enols of Substituted Cyanomalonamides. *Journal of Organic Chemistry* **2007,** 72, 5297.

[32] Ammal, S. C. and Yamataka, H., Computation Revealed a Case Where Kinetic Selectivity is Controlled by Dynamics: Isomerization of Benzylideneanilines. European *Journal of Organic Chemistry* **2006,** 2006, 4327.

[31] Ammal, S. C., Yoshikai, N., Inada, Y., Nishibayashi, Y., and Nakamura, E., Synergistic Dimetallic Effects in Propargylic Substitution Reaction Catalyzed by Thiolate-Bridged Diruthenium Complex. *The Journal of American Chemical Society* **2005,** 127, 9428.

[30] Ammal, S. C. and Yamataka, H., Linear Free Energy Relationship and Kinetic Isotope Effects as Measures for the Transition State Variation. A Case of Neophyl System. *Canadian Journal of Chemistry* **2005,** 83, 1606.

[29] Yamataka, H. Ammal, S. C., Asano, T., and Ohga, Y., Thermal Isomerization at a C=N Double Bond: How Does the Mechanism Vary with the Substituent? *Bulletin of Chemical Society of Japan* **2005,** 78, 1851.

[28] Kalaiselvan, A., Ammal, S. C., Venuvanalingam, P., and Yamataka, H., Ring Cleavage of Aziridines by Difluoroamine: Mechanistic Insights from Ab initio and DFT study. *Journal of Physical Chemistry A* **2005,** 109, 4829.

[27] Yoshikai, N., Ammal, S. C., and Nakamura, E., L-shaped Three-center Two-electron $(C\text{-}C\text{-}C)^{+}$ Bonding Array. *The Journal of American Chemical Society* **2004,** 126, 12941.

[26] Ammal, S. C., Mishima, M., and Yamataka, H., Linear Free Energy Relationship and Kinetic Isotope Effects as Measures for the Transition State Variation. A Computational Study. *Journal of Organic Chemistry* **2003,** 68, 7772.

[25] Yamataka, H. and Ammal, S. C., Nitroalkane anomaly: computational study with cluster and continuum modeling. *ARKIVOC* **2003**, 10, 59.

[24] Ammal, S. C., Yamataka, H., Aida, M., and Dupuis, M., Dynamics-Driven Reaction Pathway in an Intramolecular Rearrangement. *Science* **2003**, 299, 1555.

[23] Belosludov, R., Ammal, S. C., Inaba, Y., Oumi, Y., Takami, S., Kubo, M., Miyamoto, A., Kawasaki, M., Yoshimoto, M., and Koinuma, H., Combinatorial Computational Chemistry Approach to the Design of Metal Oxide Electronics Materials. *Proceedings of SPIE* **2000,** 3941, 2.

[22] Endou, A., Little, T. W., Yamada, A., Teraishi, K., Kubo, M., Ammal, S. C., Miyamoto, A., Kitajima, M., and Ohuchi, F. S., Chemical Interaction of NF3 with Si (Part-II): Density Functional Calculation Studies. *Surface Science* **2000,** 445, 243.

[21] Yajima, K., Ueda, Y., Tsuruya, H., Kanougi, T., Oumi, Y., Ammal, S. C., Takami, S., Kubo, M., and Miyamoto, A., Computer-Aided Design of Novel Heterogeneous Catalysts - A Combinatorial Computational Chemistry Approach. *Studies in Surface Science and Catalysis* **2000,** 130, 401.

[20] Ammal, S. C. and Venuvanalingam**,** P., Origin and Nature of Lithium and Hydrogen Bonds to Oxygen, Sulfur and Selenium. *Journal of Physical Chemistry A* **2000,** 104, 10859.

[19] Ammal, S. C. and Venuvanalingam**,** P., Ab initio and DFT Studies on the Lithium and Hydrogen Bonded Complexes of LiF and HF with σ and n+σ Donors. *Indian Journal of Chemistry A* **2000,** 39, 80.

[18] Yajima, K., Ueda, Y., Tsuruya, H., Kanougi, T., Oumi, Y., Ammal, S. C., Takami, S., Kubo, M., and Miyamoto, A., Combinatorial computational chemistry approach to the design of deNOx catalysts. *Applied Catalysis A: General* **2000,** 194-195, 183.

[17] Endou, A., Yin**,** X., Oumi, Y., Kubo, M., Teraishi, K., Ammal, S. C., and Miyamoto, A., Application of Periodic Density Functional Method to Catalyst Design. *Advances in Science and Technology* **1999,** 18, 271.

[16] Yamada, A., Endou, A., Takaba, H., Teraishi, K., Ammal, S. C., Kubo, M., Nakamura, K. G., Kitajima, M., and Miyamoto, A., Tight-binding Molecular Dynamics Simulation of Desorbed SiO Molecule during the Oxidation of Si(111) Surface. *Japanese Journal of Applied Physics* **1999**, 38, 2434.

[15] Oumi, Y., Takaba, H., Ammal, S. C., Kubo, M., Teraishi, K., Miyamoto, A., Kawasaki, M., Yoshimoto, M., and Koinuma, H., Periodic Boundary Quantum Chemical Study on ZnO Ultra-Violet Laser Emitting Materials. *Japanese Journal of Applied Physics* **1999,** 38, 2603.

[14] Onozu, T., Gunji, I., Miura, R., Ammal, S. C., Kubo, M., Teraishi, K., Miyamoto, A., Iyechika, Y., and Maeda, T., Computational Studies on GaN Surface Polarity and InN/GaN Heterostructures by Density Functional Calculations. *Japanese Journal of Applied Physics* **1999,** 38, 2544.

[13] Yin**,** X., Han, H., Gunji, I., Endou, A., Ammal, S. C., Kubo, M., and Miyamoto, A., NH_3 Adsorption on the Brönsted and Lewis Acid Sites of V_2O_5 (010): A Periodic Density Functional Study. *Journal of Physical Chemistry B* **1999,** 103, 4701.

[12] Yin**,** X., Fahmi, A., Han, H., Endou, A., Ammal, S. C., Kubo, M., Teraishi, K., and Miyamoto, A., Adsorption of H_2O on the V_2O_5 (010) Surface Studied by Periodic Density Functional Calculations. *Journal of Physical Chemistry B* **1999,** 103, 3218.

[11] Shrivastava, K. N., Ammal, S. C., Tsuruya, H., Takami, S., Endou, A., Kubo, M., Teraishi, K., Miyamoto, A., and Ozaki, A., Density Functional Theory Calculations of Molecular Nitrogen on a Ruthenium Cluster. *Chemical Physics Letters* **1999,** 313, 279.

[10] Ammal, S. C., Takami, S., Kubo, M., and Miyamoto, A., "Integrated Computational Chemistry System for Catalyst Design. *Bulletin of Material Science* **1999,** 22, 851.

[9] Buemi, G., Zuccarello, F., Venuvanalingam, P., Ramalingam, M., and Ammal, S. C. Ab Initio Study of Formazan and 3-Nitro-Formazan. *Journal of Chemical Society: Faraday Transactions* **1998,** 94, 3313.

[8] Ammal, S. C. and Venuvanalingam**,** P., π- Systems as Lithium/Hydrogen Bond Acceptors: Some theoretical Observations. *Journal of Chemical Physics* **1998,** 109, 9820.

[7] Ammal, S. C. and Venuvanalingam**,** P., Ab Initio and DFT Investigations on Lithium/Hydrogen Bonded Complexes of Trimethylamine Dimethyl ether and Dimethyl sulfide. *Journal of Chemical Society: Faraday Transactions* **1998,** 94, 2669.

[6] Ammal, S. C, Ananthavel, S. P., Venuvanalingam**,** P., and Hegde, M. S., Structure of the Benzene...ICl Complex: An UVPES and Ab Initio Molecular Orbital Study. *Journal of Physical Chemistry A* **1998,** 102, 532.

[5] Ammal, S. C., Venuvanalingam**,** P., and Pal, S. Lithium Bonding Interaction in $H_2CY...LiF$ (Y=O,S) Complexes: A Theoretical Probe. *Journal of Chemical Physics* **1997,** 107, 4329-4336.

[4] Ammal, S. C, Ananthavel, S. P., Venuvanalingam**,** P., and Hegde, M. S., UVPES and ab initio Molecular Orbital studies on the Electron Donor Acceptor Complexes of Bromine with Methylamines. *Journal of Physical Chemistry A* **1997,** 101, 1155-1159.

[3] Ammal, S. C, Ananthavel, S. P., Chandrasekhar, J., Venuvanalingam**,** P., and Hegde, M. S., Electron Donor Acceptor Complexes of Iodine with Diethyl Ether and Diethyl Sulphide - An ab initio MO Study. *Chemical Physics Letters* **1996,** 248, 153-157.

[2] Ammal, S. C. and Venuvanalingam**,** P., Local Symmetry and Coset Representations. *Chemistry Education* **1995,** 10, 4-11.

[1] Ananthavel, S. P., Ammal, S.C., Venuvanalingam**,** P., Chandrasekhar, J., and Hegde, M. S. Ultraviolet Photoelectron Spectroscopy of Complexes of Bromine with n-donors in the Vapour Phase. *Chemical Physics Letters* **1994**, 228, 431-435.

CONTRIBUTED PRESENTATIONS

[33] Contributed Talk – "Multiscale Modeling of the Electrochemical H_2 Oxidation at the Ni/YSZ Interface in the Presence and Absence of Sulfur", S. C. Ammal (presenter), A. Heyden, NAM, Louisville, KY, June 2013.

[32] Contributed Talk – "First Principles Based Microkinetic Model of the Water-Gas Shift Reaction at the Three-Phase Boundary of Pt/TiO_2 Catalysts", A. Heyden (presenter), S. C. Ammal, NAM, Louisville, KY, June 2013.

[31] Contributed Talk – "Theoretical Investigation of H_2 Oxidation on the $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ (001) Perovskite Surface under Anodic Solid Oxide Fuel Cell Conditions," A. Heyden (presenter), S. Suthirakun, S. C. Ammal, ACS Spring Meeting, New Orleans, LA, April 2013.

[30] Contributed Talk – "Multiscale Modeling of H_2 Electro-Oxidation at the Ni/YSZ Interface in the Presence and Absence of Sulfur," A. Heyden (presenter), S. C. Ammal, ACS Spring Meeting, New Orleans, LA, April 2013.

[29] Contributed Talk – "Combined DFT and Microkinetic Modeling Study of the Water-Gas Shift Reaction at the Three Phase Boundary of Pt/TiO_2 Catalysts," S. C. Ammal (presenter), A. Heyden, AIChE Annual Meeting, Pittsburgh, PA, October 2012.

[28] Contributed Talk – "Multiscale Modeling of the H_2 Oxidation Reaction at the Ni/YSZ Interface in the Presence and Absence of Sulfur," S. C. Ammal (presenter), A. Heyden, AIChE Annual Meeting, Pittsburgh, PA, October 2012.

[27] Contributed Talk – "Theoretical Investigation of the Water-Gas Shift Reaction at the Three-Phase Boundary of Ceria (111) Supported Platinum Clusters," S. Aranifard (presenter), S. C. Ammal, A. Heyden, AIChE Annual Meeting, Pittsburgh, PA, October 2012.

[26] Contributed Talk – "Theoretical Investigation of the H_2 Oxidation on the $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ (001) Perovskite Surface under Anodic Solid Oxide Fuel Cell Conditions," S. Suthirakun, S. C. Ammal, A. Heyden (presenter), AIChE Annual Meeting, Pittsburgh, PA, October 2012.

[25] Contributed Poster – "Theoretical Investigation of the Three-Phase Boundary of Ceria (111) Supported Platinum Clusters for the Water-Gas Shift Reaction," S. Aranifard (presenter), S. C. Ammal, A. Heyden, AIChE Annual Meeting, Pittsburgh, PA, October 2012.

[24] Contributed Talk – "Multiscale Modeling of the H_2 oxidation reaction at the Ni/YSZ interface in the presence and absence of sulfur," S. C. Ammal, A. Heyden (presenter), ECS PRiME Meeting, Honolulu, HI, October 2012.

[23] Contributed Talk – "Obtaining Mixed Ionic/Electronic Conductivity in Perovskite Oxides at Anodic Solid Oxide Fuel Cell Conditions: A Computational Approach," S. Suthirakun (presenter), S. C. Ammal, A. Heyden, ECS PRiME Meeting, Honolulu, HI, October 2012.

[22] Contributed Talk – "Theoretical Investigation of the H_2 Oxidation on the $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ (001) Perovskite Surface under Anodic Solid Oxide Fuel Cell Conditions," S. Suthirakun (presenter), S. C. Ammal, A. Heyden, ECS PRiME Meeting, Honolulu, HI, October 2012.

[21] Contributed Talk – "$SrTiO_3$ based Anode Materials for Solid Oxide Fuel Cells: A Computational Attempt to Understanding and Improving Performance," S. Suthirakun (presenter), S. C. Ammal, A. Heyden, AIChE Annual Meeting, Minneapolis, MN, October 2011.

[20] Contributed Talk – "Multiscale Modeling of the Water-Gas Shift Reaction at the Three Phase Boundary of Pt/TiO_2 and Pt/CeO_2 Catalysts," S. C. Ammal, S. Aranifard, A. Heyden (presenter), AIChE Annual Meeting, Minneapolis, MN, October 2011.

[19] Contributed Poster – "Theoretical Investigation of the Three-Phase Boundary of Ceria (111) Supported Platinum Clusters for the Water-Gas Shift Reaction," S. Aranifard (presenter), S. C. Ammal, A. Heyden, SECS Annual Meeting, Asheville, NC, September 2011 – 3rd price poster award.

[18] Contributed Talk – "Multiscale Modeling of the Water-Gas Shift Reaction at the Three Phase Boundary of Pt/TiO_2 Catalysts," A. Heyden (presenter), S. C. Ammal, SECS Annual Meeting, Asheville, NC, September 2011.

[17] Contributed Talk – "Density Functional Theory Study on the Electronic Structure of n- and p-type Doped $SrTiO_3$ as Anode for Solid Oxide Fuel Cells," S. Suthirakun (presenter), S. C. Ammal, A. Heyden, SECS Annual Meeting, Asheville, NC, September 2011.

[16] Contributed Talk – "Multiscale Modeling of the Water-Gas Shift Reaction at the Three Phase Boundary of Pt/TiO_2 Catalysts," A. Heyden (presenter), S. C. Ammal, EuropaCat X, Glasgow, Scotland, August 2011.

[15] Contributed Poster – "$SrTiO_3$ based Anode Materials for Solid Oxide Fuel Cells: A Computational Attempt to Understanding and Improving Performance," S. Suthirakun, S. C. Ammal, A. Heyden (presenter), EuropaCat X, Glasgow, Scotland, August 2011.

[14] Contributed Poster – "Theoretical Investigation of the Three-Phase Boundary of Ceria (111) Supported Platinum Clusters for the Water-Gas Shift Reaction," S. Aranifard, S. C. Ammal, A. Heyden (presenter), EuropaCat X, Glasgow, Scotland, August 2011.

[13] Contributed Talk – "Multiscale Modeling of the Water-Gas Shift Reaction at the Three Phase Boundary of Pt/TiO_2 Catalysts," A. Heyden (presenter), S. C. Ammal, NAM, Detroit, MI, June 2011.

[12] Contributed Poster – "Theoretical Investigation of the Three-Phase Boundary of Ceria (111) Supported Platinum Clusters for the Water-Gas Shift Reaction," S. Aranifard (presenter), S. C. Ammal, A. Heyden, NAM, Detroit, MI, June 2011.

[11] Contributed Poster – "$SrTiO_3$ based Anode Materials for Solid Oxide Fuel Cells: A Computational Attempt to Understanding and Improving Performance," S. Suthirakun (presenter), S. C. Ammal, A. Heyden, NAM, Detroit, MI, June 2011.

[10] Contributed Poster – "Theoretical Investigation of Oxygen Ion Transport in Doped Perovskite and Double Perovskite Structures of $SrTiO_3$ and $Sr_2Fe_{1.5}Mo_{0.5}O_6$ for Solid Oxide Fuel Cell Applications," S. Suthirakun (GS presenter), S. C. Ammal, A. Heyden, AIChE Annual Meeting, Salt Lake City, UT, November 2010.

[9] Contributed Poster – "Theoretical Investigation of the Three-Phase Boundary of Ceria Supported Noble Metal Clusters," S. Aranifard (GS presenter), S. C. Ammal, A. Heyden, AIChE Annual Meeting, Salt Lake City, UT, November 2010.

[8] Contributed Talk – "Multiscale Modeling of Bifunctional Catalysts for the Water-Gas Shift Reaction," A. Heyden (presenter), S. C. Ammal, 21st International Symposium of Chemical Reaction Engineering, Philadelphia, PA, June 2010.

[7] Contributed Talk – "Theoretical Investigation of the Water-Gas Shift Reaction at the Three-Phase Boundary of TiO2 Supported Metal Clusters," A. Heyden (presenter), S. C. Ammal, AIChE Annual Meeting, Nashville, TN, November 2009.

[6] Contributed Talk – "Theoretical Investigation of the Water-Gas Shift Reaction at the Three-Phase Boundary of TiO2 Supported Metal Clusters," S. C. Ammal (presenter), A. Heyden, ACS Fall National Meeting, Washington, DC, August 2009.

[5] Contributed Talk – "Ab initio Molecular Dynamics Simulations of Intramolecular Rearrangement Reaction of Pinacolyl Alcohol," S. C. Ammal (presenter) and H. Yamataka, Kyushu International Symposium on Physical Organic Chemistry (KISPOC-IX), Fukuoka (Japan): Nov. 27-30, 2001.

[4] Contributed Poster – "Quantum Chemical Study on the Surface Structure and Doping of ZnO. An Ultra-Violet Laser Emitting Material," Y. Oumi, H. Takaba, S. C. Ammal (presenter), M. Kubo, K. Teraishi, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and K. Koinuma, 5th International Workshop on Oxide Electronics, University of Maryland (USA): Dec.7-8, 1998.

[3] Contributed Talk – "Quantum Molecular Dynamics Study on the Oxidation of Si Surface," K. Teraishi, S. C. Ammal (presenter), A. Yamada, A. Endou, M. Kubo, and A. Miyamoto,, MRS Fall Meeting 98, Boston, MA, Nov. 30 – Dec. 4, 1998.

[2] Contributed Talk – "Periodic Boundary Quantum Chemical Study on ZnO Ultra-Violet Laser Emitting Materials," Y. Oumi, H. Takaba, S. C. Ammal (presenter), M. Kubo, K. Teraishi, A. Miyamoto, M. Kawasaki, M. Yoshimoto, and K. Koinuma, International Conference on Solid State Devices and Materials (SSDM)', Hiroshima (Japan): Sept. 7-10, 1998.

[1] Contributed Talk – "Origin and Nature of Lithium and Hydrogen Bonding Interactions with n-donors," S. C. Ammal (presenter) and P. Venuvanalingam, International Conference on Molecular Association, Aligarh Muslim University, Aligarh (India): March 18-20, 1996.