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WORK ADDRESS

School of Molecular Sciences (Formerly Department of Chemistry & Biochemistry)
Arizona State University
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EDUCATION

Ph.D., Indian Institute of Technology, Kanpur, India, **1994**, Chemistry

M. Sc., University of Roorkee, Roorkee, India, **1988**, Chemistry

B. Sc., Orissa University of Agriculture and Technology, India, **1986**, Chemistry

SUMMARY OF EXPERIENCE

I have 25 years of teaching and research experience in several areas of contemporary interest in computational chemistry, material design, nanotechnology, catalysis, and energy related research. I am one of the pioneers in the detailed theoretical characterization of weak van der Waals interactions and their manifestations in nanomaterial design and spectroscopic characterization of large biomolecular complexes. In recent years, my research has focused on computational investigations of interfaces and their role in modulating charge-transfer in surface-enhanced Raman scattering, dye-sensitized solar cells, photocatalysis, and biophotovoltaics. In the pharma industry, my research was focused on developing novel therapeutic agents against the macrophage based infectious diseases, viz., tuberculosis, leprosy, and leishmaniasis.

EMPLOYMENT

Arizona State University, Jan. 2010 – Present, Associate Research Professor (Graduate Faculty), Research Faculty

University of Nevada, Las Vegas, Mar. 2007 – Dec. 2009, Research Assistant Professor (Graduate Faculty)

Korea Institute for Advanced Study, Seoul, Korea, Oct. 2003 – Feb. 2007, KIAS Assistant Professor

Pohang University of Science and Technology, Korea, Jan. 1997 – Sep. 2003, Research Associate Professor, Research Assistant Professor, Research Scientist, Postdoctoral Fellow

Torrent Pharmaceuticals, Ahmedabad, India, Sep. 1994 – Dec. 1996, Scientist – I, Research Associate (Drug Design)

TEACHING

Courses Teaching/Taught

CHM 433/531 (Advanced Organic Chemistry I), Fall-2011, Fall-2014)

CHE 122 (General Chemistry II, Summer 2009)

CHE 402/602 (Scientific Software), Fall 2007)

PUBLICATIONS

Refereed Journal Articles – (Google Scholar ~ 6276 citations: H-index: 41)

1. Electrochemical Capture and Release of Carbon Dioxide, J. H. Rheinhardt, P. Singh, **P. Tarakeshwar**, and D. A. Buttry, *ACS Energy Lett.* **2** (2017) 454-461.
2. Electrochemical Capture and Release of Carbon Dioxide Using a Disulfide-Thiocarbonate Redox Cycle, P. Singh, J. H. Rheinhardt, J. Z. Olson, **P. Tarakeshwar**, V. Mujica, and D. A. Buttry, *J. Am. Chem. Soc. Commun.* **139** (2017) 1033-1036.
3. Polarizability as a Molecular Descriptor for Conductance in Organic Molecular Circuits, S. K.S. Mazinani, R. V. Meidanshahi, J. L. Palma, **P. Tarakeshwar**, T. Hansen, M. A. Ratner, and V. Mujica, *J. Phys. Chem. C* **120** (2016) 26054-26060.
4. Single-Molecule Conductance through Hydrogen Bonds: The Role of Resonances, M. Wimmer, J. L. Palma, **P. Tarakeshwar**, and V. Mujica, *J. Phys. Chem. Lett.* **7** (2016) 2977-2980.
5. Pseudocarbynes: Charge-Stabilized Carbon Chains, **P. Tarakeshwar**, P. R. Buseck, and H. W. Kroto, *J. Phys. Chem. Lett.* **7** (2016) 1675-1681. (Work highlighted in Chem&Engg. News, http://cen.acs.org/articles/94/i20/Harry-Krotos-last-words-carbyne.html).
6. Solvent Effects on the Dynamic Polarizability and Raman Response of Hybrid Molecule-Metal Oxide Nanoparticles, Y. Orozco-Gonzalez, **P. Tarakeshwar**, S. Canuto, and V. Mujica, *ChemPhysChem* **17** (2016) 2590-2595.

7. A Nickel Phosphine Complex as a Fast and Efficient Hydrogen Production Catalyst, L. Gan, T. L. Groy, **P. Tarakeshwar**, S. K. S. Mazinani, J. Shearer, V. Mujica, and A. K. Jones, *J. Am. Chem. Soc.* **137** (2015) 1109-1115.

8. Electronic Transport across Hydrogen Bonds in Organic Electronics, R. V. Meidanshahi, S. K. S. Mazinani V. Mujica, and **P. Tarakeshwar**, *Int. J. Nanotechnol.* **12** (2015) 297-312.

9. Probing the Nature of Charge Transfer at Nano-Bio Interfaces: Peptides on Metal Oxide Nanoparticles, **P. Tarakeshwar**, J. L. Palma, G. P. Holland, P. Fromme, J. L. Yarger, and V. Mujica, *J. Phys. Chem. Lett.* **5** (2014) 3555-3559.

10. Dopamine Adsorption on TiO_2 Anatase Surfaces, I. Urdaneta, A. Keller, O. Atabek, J. L. Palma, D. Finkelstein-Shapiro, **P. Tarakeshwar**, V. Mujica, and M. Calatayud, *J. Phys. Chem. C*, **118** (2014), 20688–20693.

11. Catalytic hydrogen evolution by Fe(II) carbonyls featuring a dithiolate and a chelating phosphine, S. Roy, S. K. S. Mazinani, T. L. Groy, L. Gan, P. Tarakeshwar, V. Mujica, and A. K. Jones, *Inorg. Chem.* **53** (2014) 8919-8929.

12. SERS as a Probe of Charge-transfer Pathways in Hybrid Dye/Molecule-metal Oxide Complexes, **P. Tarakeshwar**, J. L. Palma, D. Finkelstein-Shapiro, A. Keller, I. Urdaneta, M. Calatayud, O. Atabek, and V. Mujica, *J. Phys. Chem. C* **118** (2014) 3774-3782.

13. Probing Raman enhancement in a Dopamine-Ti_2O_4 hybrid using stretched molecular geometries, I. Urdaneta, J. Pilmé, A. Keller, O. Atabek, **P. Tarakeshwar**, V. Mujica, and M. Calatayud, *J. Phys. Chem. A* **118** (2014) 1196-1202.

14. Chemically induced magnetism in atomically precise gold clusters, K. S. Krishna, **P. Tarakeshwar**, V. Mujica, and C. S. S. R. Kumar, *Small* **10** (2014) 907-911.

15. Vibrational signatures of Watson-Crick base pairing in adenine-thymine mimics, Y. Nosenko, M. Kunitski, T. Stark, M. Göbel, **P. Tarakeshwar** and B. Brutschy, *Phys. Chem. Chem. Phys.* **15** (2013) 11520-11530.

16. CO_2 pre-activation in photo-induced reduction via surface functionalization of TiO_2 nanoparticles, D. Finkelstein-Shapiro, S. J. Hurst-Petrosko, N. Dimitrijevic, D. Gosztola, K. A. Gray, T. Rajh, **P. Tarakeshwar**, and V. Mujica, *J. Phys. Chem. Lett.* **4** (2013) 475-479.

17. Simple and accurate correlation of experimental redox potentials and DFT-calculated HOMO/LUMO energies of polycyclic aromatic hydrocarbons, D. D. Méndez-Hernández, **P. Tarakeshwar**, D. Gust, T. A. Moore, A. L. Moore, and V. Mujica, *J. Mol. Model.* **19** (2013) 2845-2848.

18. The Stability and Quenching of Plasmon Resonance Absorption in Magnetic Gold Nanoparticles, A. Roldan, F. Illas, **P. Tarakeshwar**, and V. Mujica, *J. Phys. Chem. Lett.* **2** (2011) 2996-3001.

19. 4-Aminobenzimidazole:1-Methylthymine: a model for investigating Hoogsteen base-pairing between Adenine and Thymine, Y. Nosenko, M. Kunitski, T. Stark, M. Göbel, **P. Tarakeshwar**, and B. Brutschy, *J. Phys. Chem. A* **115** (2011) 11403–11411.

20. SERS on semiconducting oxide nanoparticles: Oxide nature, size, solvent, and pH effects, **P. Tarakeshwar**, D. Finkelstein-Shapiro, S. J. Hurst, T. Rajh, and V. Mujica, *J. Phys. Chem. C* **115** (2011) 8994-9004.

21. Quantum Confinement Effects on the Surface Enhanced Raman Spectra of Hybrid Systems Molecule-TiO_2 Nanoparticles, **P. Tarakeshwar**, D. Finkelstein-Shapiro, T. Rajh, and V. Mujica, ***Int. J. Quant. Chem.* 111** (2011) 1659-1670.

22. Photo-Induced Kinetics of SERS in Bio-Inorganic Hybrid Systems. A Case Study: Dopamine-TiO_2, D. Finkelstein-Shapiro, **P. Tarakeshwar**, T. Rajh, and V. Mujica, ***J. Phys. Chem. B* 114** (2010) 14642-14645.

23. Exploring Gas Phase Ion-Ionophore Interactions: IR Spectroscopy of Argon-Tagged Alkali Ion-Crown Ether Complexes, J. Rodriguez, D. Kim, **P. Tarakeshwar**, and J. Lisy, ***J. Phys. Chem. A* 114** (2010) 1514-1520.

24. Pseudorotation in pyrrolidine: rotational coherence spectroscopy and ab initio calculations of a large amplitude intramolecular motion, M. Kunitski, C. Riehn, V. V. Matylitsky, **P. Tarakeshwar**, and B. Brutschy, ***Phys. Chem. Chem. Phys.* 12** (2010) 72-81.

25. Geometric and electronic structures of hydrogenated transition metal (Sc, Ti, Zr) clusters, T. J. Dhilip Kumar, **P. Tarakeshwar**, and N. Balakrishnan, ***Phys. Rev. B* 79** (2009) 205415.

26. Hydrogen Multicenter Bonds and Reversible Hydrogen Storage, **P. Tarakeshwar**, T. J. Dhilip Kumar, and N. Balakrishnan, ***J. Chem. Phys.* 130** (2009) 114301.

27. Electrode-Molecule Interface Effects on Molecular Conductance, **P. Tarakeshwar**, J. J. Palacios, and D. M. Kim, ***IEEE Trans on Nanotech.* 8** (2009) 16-21.

28. Structural, energetic, and electronic properties of hydrogenated titanium clusters, T. J. Dhilip Kumar, **P. Tarakeshwar**, and N. Balakrishnan, ***J. Chem. Phys.* 124** (2008) 194714.

29. Nature of Hydrogen Interaction and Saturation on Small Titanium Clusters, **P. Tarakeshwar**, T. J. Dhilip Kumar, and N. Balakrishnan, ***J. Phys. Chem. A* 112** (2008) 2846-2854.

30. Metal contacts in carbon nanotube field-effect transistors: Beyond the Schottky barrier paradigm, J. J. Palacios, **P. Tarakeshwar**, and D. M. Kim, ***Phys. Rev. B* 77** (2008) 113403.

31. Interface Study of Metal Electrode and Semiconducting Carbon Nanotubes: Effects of Electrode Atomic Species, **P. Tarakeshwar**, J. J. Palacios, and D. M. Kim, ***IEEE Trans on Nanotech.* 7** (2008) 124-127.

32. Supersonic jet studies of solvation effects on spectroscopy and photophysics of 4-diethylaminopyridine, I. Szydlowska, Y. Nosenko, B. Brutschy, **P. Tarakeshwar**, and J. Herbich, ***Phys. Chem. Chem. Phys.* 9** (2007) 4981-4991.

33. Cation-π-anion interaction: A theoretical investigation of the role of induction energies, D. Kim, E. C. Lee, K. S. Kim, and **P. Tarakeshwar**, ***J. Phys. Chem. A* 111** (2007) 7980-7986.

34. Understanding of Assembly Phenomena by Aromatic-Aromatic Interactions: Benzene Dimer and the Substituted Systems, E. C. Lee, D. Kim, P. Jurečka, **P. Tarakeshwar**, P. Hobza, and K. S. Kim, ***J. Phys. Chem. A* 111** (2007) 3446-3457. (**Feature Article**)

35. Structures, energetics, and spectra of aqua-cesium (I) complexes: An ab initio and experimental study, M. Kołaski, H. M. Lee, Y. C. Choi, K. S. Kim, **P. Tarakeshwar**, D. J. Miller, and J. M. Lisy, ***J. Chem. Phys.* 126** (2007) 074302.

36. Hydration Profiles of Aromatic Amino Acids: Conformations and Vibrations of *L*-Phenylalanine-$(H_2O)_n$ Clusters, T. Ebata, T. Hashimoto, T. Ito, Y. Inokuchi, F. Altunsu, B. Brutschy, and **P. Tarakeshwar**, ***Phys. Chem. Chem. Phys.*** 8 (2006) 4783-4791. (**Cover Article**)

37. Hydration and dissociation of hydrogen fluoric acid (HF), S. Odde, B. J. Mhin, K. H. Lee, H. M. Lee, **P. Tarakeshwar**, and K. S. Kim, ***J. Phys. Chem. A* 110** (2006) 7918-7924.

38. Modulation of Molecular Conductance Induced by Electrode Atomic Species and Interface Geometry, **P. Tarakeshwar**, J. J. Palacios, and D. M. Kim, ***J. Phys. Chem. B* 110** (2006) 7456-7462.

39. Characterization of Weak NH-π Intermolecular Interactions of Ammonia with various Substituted π Systems, S. Vaupel, B. Brutschy, **P. Tarakeshwar**, and K. S. Kim, ***J. Am. Chem. Soc.* 128** (2006) 5416-5426.

40. Study of Interactions of Various Ionic Species with Solvents Toward the Design of Receptors, N. J. Singh, A. C. Olleta, Anupriya, M. Park, H. -B. Yi, I. Bandyopadhyay, H. M. Lee, **P. Tarakeshwar**, and K. S. Kim, ***Theor. Chem. Acc.* 115** (2006) 127-135.

41. Why the hydration energy of Au^+ is larger for the second water molecule than the first one: Skewed orbitals overlap, H. M. Lee, M. Diefenbach, S. B. Suh, **P. Tarakeshwar**, and K. S. Kim, ***J. Chem. Phys.* 123** (2005) 074328.

42. Modulation of the Electronic Structure of Semiconducting Nanotubes resulting from Different Metal Contacts, P. Tarakeshwar, and D. M. Kim, ***J. Phys. Chem. B* 109** (2005) 7601-7604.

43. Substituent Effects on the Edge-to-Face Aromatic Interactions, E. C. Lee, B. H. Hong, J. Y. Lee, J. C. Kim, D. Kim, Y. Kim, **P. Tarakeshwar**, and K. S. Kim, ***J. Am. Chem. Soc.* 127** (2005) 4530-4537.

44. Role of molecular orbitals of the benzene in electronic nano-devices, Y.-C. Choi, W. Y. Kim, K.-S. Park, **P. Tarakeshwar**, K. S. Kim, T.-S. Kim, and J. Y. Lee, ***J. Chem. Phys.* 122** (2005) 094706.

45. Origin of the magic numbers of water clusters with an excess electron, H. M. Lee, S. B. Suh, **P. Tarakeshwar**, and K. S. Kim, ***J. Chem. Phys.* 122** (2005) 044309.

46. Structures, energetics, and spectra of hydrated hydroxide anion clusters, H. M. Lee, **P. Tarakeshwar**, and K. S. Kim, ***J. Chem. Phys.* 121** (2004) 4657-4664.

47. *p*-benzoquinone-benzene clusters as potential nanomechanical devices: A theoretical study, T. K. Manojkumar, H. S. Choi, B. H. Hong, **P. Tarakeshwar**, and K. S. Kim, ***J. Chem. Phys.* 121** (2004) 841-846.

48. Insights into the Structures, Energetics, and Vibrations of Monovalent Cation-$(Water)_{1-6}$ Clusters, H. M. Lee, **P. Tarakeshwar**, J. Park, M. R. Kolaski, Y. J. Yoon, H.-B. Yi, W. Y. Kim and K. S. Kim, ***J. Phys. Chem. A* 108** (2004) 2949-2958.

49. Theoretical investigations of anion-π interactions: The role of anions and the nature of π systems, D. Kim, **P. Tarakeshwar**, and K. S. Kim, ***J. Phys. Chem. A* 108** (2004) 1250-1258.

50. Insights into the structure of cyclohexane from femtosecond degenerate four-wave mixing spectroscopy and ab initio calculations, C. Riehn, V. V. Matylitsky, W. Jareba, B. Brutschy, **P. Tarakeshwar**, and K. S. Kim, ***J. Am. Chem. Soc.* 125** (2003) 16455-16462.

51. Structures, energies, and spectra of aqua-silver (I) complexes, E. C. Lee, H. M. Lee, **P. Tarakeshwar**, and K. S. Kim, ***J. Chem. Phys.* 119** (2003) 7725-7736.

52. Geometrical and electronic structures of gold, silver, and gold-silver binary clusters: Origins of ductility of gold and gold-silver alloy formation, H. M. Lee, M. Ge, B. R. Sahu, **P. Tarakeshwar**, and K. S. Kim, ***J. Phys. Chem. B* 107** (2003) 9994-10005.

53. Highly stereospecific epimerization of α-amino acids: Conducted tour mechanism, I. Bandyopadhyay, H. M. Lee, **P. Tarakeshwar**, C. Cui, K. S. Oh, J. Chin, and K. S. Kim, ***J. Org. Chem.* 68** (2003) 6571-6575.

54. Electronic structure of silver subnanowires in self-assembled organic nanotubes: First principles calculations, S. B. Suh, B. H. Hong, **P. Tarakeshwar**, S. J. Youn, S. Jeong and K. S. Kim, ***Phys. Rev. B*** *Rapid Commun.* **67** (2003) 241402(R).

55. Ab initio studies of neutral and anionic p-benzoquinone-water clusters, T. K. Manojkumar, H. S. Choi, **P. Tarakeshwar**, and K. S. Kim, ***J. Chem. Phys.* 118** (2003) 8681-8686.

56. Cation-π interactions: A theoretical investigation of the interaction of metallic and organic cations with alkenes, arenes, and heteroarenes, D. Kim, S. Hu, **P. Tarakeshwar**, K. S. Kim, and J. M. Lisy, ***J. Phys. Chem. A* 107** (2003) 1228-1238.

57. An electrochemically controllable nanomechanical molecular system utilizing edge-to-face and face-to-face aromatic interactions, H. G. Kim, C.-W. Lee, S. Yun, B. H. Hong, Y.-O. Kim, D. Kim, H. Ihm, J. W. Lee, E. C. Lee, **P. Tarakeshwar**, S.-M. Park, and K. S. Kim, ***Org. Lett.* 4** (2002) 3971-3974.

58. Assembling phenomena of calix[4]hydroquinone nanotube bundles by one-dimensional short hydrogen bonding and displaced π-π stacking, K. S. Kim, S. B. Suh, J. C. Kim, B. H. Hong, E. C. Lee, S. Yun, **P. Tarakeshwar**, J. Y. Lee, Y. Kim, H. Ihm, H. G. Kim, J. W. Lee, J. K. Kim, H. M. Lee, D. Kim, C. Cui, S. J. Youn, H. Y. Chung, H. S. Choi, C.-W. Lee, S. J. Cho, S. Jeong, and J.-H. Cho, ***J. Am. Chem. Soc***. **124** (2002) 14268-14279.

59. Anisole-$(H_2O)_n$ (n=1-3) complexes: An experimental and theoretical investigation of the modulation of optimal structures, binding energies and vibrational spectra in both the ground and first excited states, B. Reimann, K. Buchhold, H.-D. Barth, B. Brutschy, **P. Tarakeshwar** and K. S. Kim, ***J. Chem. Phys.* 117** (2002) 8805-8822.

60. Insights into the nature of SiH_4-BH_3 complex: A theoretical investigation of new mechanistic pathways involving $SiH_3^{\cdot}$ and $BH_4^{\cdot}$ radicals, S. Hu, J. Kim, **P. Tarakeshwar**, and K. S. Kim, ***J. Phys. Chem. A* 106** (2002) 6817-6822.

61. Comparison of the nature of π and conventional H-bonds: A theoretical investigation, **P. Tarakeshwar** and K. S. Kim, ***J. Mol. Str.* 615** (2002) 227-238.

62. Nature of the interaction of paramagnetic atoms (A=^{4}N, ^{4}P, ^{3}O, ^{3}S) with π systems and C_{60}: A theoretical investigation of A$\cdots C_6H_6$ and endohedral fullerenes A@C_{60}, J. M. Park, **P. Tarakeshwar**, K. S. Kim, and T. Clark, ***J. Chem. Phys.* 116** (2002) 10684-10691.

63. Catalytic mechanism of enzymes: Preorganization, short strong hydrogen bond, and charge buffering, K. S. Kim, D. Kim, J. Y. Lee, **P. Tarakeshwar**, and K. S. Oh, ***Biochem.* 41** (2002) 5300-5306.

64. A New Type of Ionophore Family Utilizing the Cation-Olefinic π Interaction: Theoretical Study of [*n*]Beltenes**,** H. S. Choi, D. Kim, **P. Tarakeshwar**, S. B. Suh, and K. S. Kim, ***J. Org. Chem.* 67** (2002), 1848-1851.

65. On the microscopic interaction of p-chlorofluorobenzene with water, C. Riehn, B. Reimann, K. Buchhold, H.-D. Barth, S. Vaupel, B. Brutschy, **P. Tarakeshwar**, and K. S. Kim, ***J. Chem. Phys.* 115** (2001) 10045-10047.

66. Structure and stability of fluorine-substituted benzene-argon complexes: The decisive role of exchange-repulsion and dispersion interactions, **P. Tarakeshwar**, K. S. Kim, E. Kraka and D. Cremer, ***J. Chem. Phys.* 115** (2001) 6018-6029.

67. Olefinic vs. aromatic π-H interaction: A theoretical investigation of the nature of interaction of first-row hydrides with ethene and benzene, **P. Tarakeshwar**, H. S. Choi, and K. S. Kim, ***J. Am. Chem. Soc.* 123** (2001) 3323-3331.

68. Ab initio studies of π-water tetramer complexes. Evolution of optimal structures, binding energies and vibrational spectra of π-$(H_2O)_n$ (n=1-4) complexes, **P. Tarakeshwar**, K. S. Kim, S. Djafari, K. Buchhold, B. Reimann, H.-D. Barth and B. Brutschy, ***J. Chem. Phys.* 114** (2001) 4016-4024.

69. σ to π conformational transition: Interactions of the water trimer with π-systems, **P. Tarakeshwar**, K. S. Kim and B. Brutschy, ***J. Chem. Phys.* 114** (2001) 1295-1305.

70. The molecular structure of para-cyclohexylaniline. Comparison of results obtained by X-ray diffraction with gasphase laser experiments and ab initio calculations, C. Riehn, A. Degen, A. Weichert, M. Bolte, E. Egert, B. Brutschy, **P. Tarakeshwar** and K. S. Kim, ***J. Phys. Chem. A*, 104** (2000) 11593-11600.

71. Role of catalytic residues in enzymatic mechanisms of homologous *Ketosteroid Isomerases*, K. S. Oh, S.-S. Cha, D.-H. Kim, H.-S. Cho, N.-C. Ha, G. Choi, J. Y. Lee, **P. Tarakeshwar**, H. S. Son, K. Y. Choi, B.-H. Oh, and K. S. Kim, ***Biochem.* 39** (2000) 13891 - 13896.

72. Structures, vibrational frequencies, and IR spectra of hexa-hydrated benzene clusters, J. Y. Lee, J. Kim, H. M. Lee, **P. Tarakeshwar** and K. S. Kim, ***J. Chem. Phys.* 113** (2000) 6160-6168.

73. Structures, energies, vibrational spectra, and electronic properties of water monomer to decamer, H. M. Lee, S. B. Suh, J. Y. Lee, **P. Tarakeshwar** and K. S. Kim, ***J. Chem. Phys.* 112** (2000) 9759-9772, **114** (2000) 3343.

74. Dimer to monomer phase transition in alkali-metal fullerides: Magnetic susceptibility changes, K. S. Kim, J. M. Park, J. Kim, S. B. Suh, **P. Tarakeshwar**, K. H. Lee and S. S. Park, ***Phys. Rev. Lett.* 84** (2000) 2425-2428.

75. Interaction of the water dimer with π-systems: A theoretical investigation of structures, energies, and vibrational frequencies, **P. Tarakeshwar**, K. S. Kim and B. Brutschy, ***J. Chem. Phys.* 112** (2000) 1769-1781.

76. Fluorobenzene and p-difluorobenzene microsolvated by methanol: an infrared spectroscopic and ab initio theroretical investigation, K. Buchhold, B. Reimann, S. Djafari, H.-D. Barth, B. Brutschy, **P. Tarakeshwar** and K. S. Kim, ***J. Chem. Phys.* 112** (2000) 1844-1858.

77. Van der Waals isomers and ionic reactivity of the cluster system: para-Chlorofluorobenzene/Methanol, C. Riehn, K. Buchhold, B. Reimann, S. Djafari, H.-D. Barth, B. Brutschy, **P. Tarakeshwar** and K. S. Kim, ***J. Chem. Phys.* 112** (2000) 1170-1177.

78. A theoretical investigation of benzene-AlX_3 and ethene-AlX_3 (X=H,F,Cl) Interactions, **P. Tarakeshwar** and K. S. Kim, ***J. Phys. Chem. A***, **103** (1999) 9116-9124, 11486.

79. A theoretical investigation of the nature of the π-H interaction in ethene-H_2O, benzene-H_2O, and benzene-$(H_2O)_2$, **P. Tarakeshwar**, H. S Choi, S. J. Lee, J. Y. Lee, K. S. Kim, T. K. Ha, J. H. Jang, J. G. Lee, and H. Lee***, J. Chem. Phys.* 111** (1999) 5838-5850.

80. Fluorobenzene-water and difluorobenzene-water systems: An ab initio investigation, **P. Tarakeshwar**, K. S. Kim and B. Brutschy, ***J. Chem. Phys.* 110** (1999) 8501-8512.

81. An ab initio study of benzene-BX_3(X=H,F,Cl) interactions, **P. Tarakeshwar**, S. J. Lee, J. Y. Lee and K. S. Kim, ***J. Phys. Chem. B***, **103** (1999) 184-191.

82. Benzene-hydrogen halide interactions: Theoretical studies of binding energies, vibrational frequencies and equilibrium structures, **P. Tarakeshwar**, S. J. Lee, J. Y. Lee and K. S. Kim, ***J. Chem. Phys.***, **108** (1998) 7217-7223.

83. An ab initio study of pyruvic acid, **P. Tarakeshwar** and S. Manogaran, ***J. Mol. Struc. (Theochem)***, **430** (1998) 51-56.

84. Role of Lewis acid ($AlCl_3$)-aromatic ring interactions in Friedel-Craft's reaction: An ab initio study, **P. Tarakeshwar**, J. Y. Lee and K. S. Kim, ***J. Phys. Chem. A***, **102** (1998) 2253-2255.

85. Proline and hydroxyproline zwitterions--an ab initio study, **P. Tarakeshwar** and S. Manogaran***, J. Mol. Struc. (Theochem)***, **417** (1997) 255-263.

86. Vibrational frequencies of proline and hydroxyproline: An ab initio study, **P. Tarakeshwar** and S. Manogaran, ***J. Mol. Struc. (Theochem)***, **365** (1996) 167-181.

87. Conformations and vibrations of dicarboxylic acids: An ab initio study, **P. Tarakeshwar** and S. Manogaran, ***J. Mol. Struc. (Theochem)***, **362** (1996) 77-99.

88. Vibrational frequencies of cysteine and serine zwitterions—an ab initio assignment, **P. Tarakeshwar** and S. Manogaran, ***Spectrochim. Acta***, **51A** (1995) 925-928.

89. Ground state vibrations of citric acid and the citrate trianion: An ab initio study, **P. Tarakeshwar** and S. Manogaran***, Spectrochim. Acta***, **50A** (1994) 2327-2343.

90. Conformational effects on vibrational frequencies of cysteine and serine: An ab initio study, **P. Tarakeshwar** and S. Manogaran, ***J. Mol. Struc. (Theochem)***, **305** (1994) 205-224.

91. Stereoselective synthesis of substituted tetrahydrofurans: Identification and analysis by proton NMR, and MNDO, MM2 calculations, **P. Tarakeshwar**, J. Iqbal and S. Manogaran, ***Tetrahedron***, **47** (1991) 297-304.

Refereed Journal Reviews -

1. Molecular clusters of π-Systems: Theoretical studies of structures, spectra and origin of interaction energies, K. S. Kim, **P. Tarakeshwar** and J. Y. Lee, ***Chem. Rev.* 100** (2000) 4145-4186.

Book/Monograph Contributions –

1. *Nanosensors for Biomedical Applications: A Tutorial*, H. Clingan, A. Laidlaw, **P. Tarakeshwar**, M. Wimmer, A. Garcia, and V. Mujica, in, "Semiconductor Nanotechnology", Eds. S. M. Goodnick, A. Korkin, and R. Nemanich, Springer Nature, USA, 2018, 145-167.
2. *Atomically Precise Gold Catalysis*, K. S. Krishna, J. Liu, **P. Tarakeshwar**, V. Mujica, J. J. Spivey, and C. S. S. R. Kumar, Chapter 4 in "Atomically-Precise Methods for Synthesis of Solid Catalysts", RSC Catalysis Series No. 22, Eds. S. Hermans and T. V. de Bocarme, The Royal Society of Chemistry, London, U. K. 2015, 87-122.
3. *Clusters to Nanomaterials and Molecular Devices: Theoretical Exploration,* Kwang S. Kim, **P. Tarakeshwar**, and Han Myoung Lee. A contribution to the book on "Theory and Applications of Computational Chemistry: The First 40 Years, A Volume of Technical and Historical Perspectives, Eds., Clifford E. Dykstra, Gernot Frenking, Kwang S. Kim, and Gustavo Scuseria, Elsevier Science, The Netherlands, 2005, 963-993.
4. *De novo theoretical design of functional nanomaterials and molecular devices,* Kwang S. Kim, **P. Tarakeshwar**, and Han Myoung Lee. A contribution to the "Dekker Encyclopedia of Nanoscience and Nanotechnology", Eds., James A. Schwarz, Cristian Contescu and Karol Putyera, Marcel Dekker Inc., New York, 2004, 2423–2433.
5. *Theoretical Approaches to the Design of Functional Nanomaterials*, **P. Tarakeshwar**, Dongwook Kim, Han Myoung Lee, Seung Bum Suh, and Kwang S. Kim. A contribution to the 15th volume on "Theoretical Computational Chemistry (Computational Material Science)"; Ed: Jerzy Leszczynski, Elsevier Science, The Netherlands, 2004, 119-170.
6. *Nanorecognition*, **P. Tarakeshwar** and K. S. Kim, A contribution to the "Encyclopedia of Nanoscience and Nanotechnology"; Ed: H. S. Nalwa, American Science Publishers, California, 2004, Vol. 7, 367-404.
7. *Insights from theoretical investigations of aqueous clusters*, **P. Tarakeshwar**, H. M. Lee and K. S. Kim. A contribution to the festschrift volume to honor Professor R.G. Parr on his 80th birthday; Ed: K. D. Sen, World Scientific, Singapore, 2002, pp 1642-1683.

Technical Proceedings –

1. *Electronic and Vibrational Properties of Magnetic Core-Shell Nanoparticles,* A. Di Bernardo, P. Tarakeshwar, and V. Mujica, Proceedings of the 6th European Conference on Antennas and Propagation, Prague, Czech Republic, (March 20-26, 2012).
2. *Electrode-Molecule Interface Effects on Molecular Conductance,* **P. Tarakeshwar**, J. J. Palacios and D. M. Kim, Technical Proceedings of the IEEE Nanotechnology Materials and Devices Conference 2006, 156-157 (2006).
3. *Interface Study of Metal Electrode and Semiconducting Carbon Nanotubes: Effects of Electrode Atomic Species,* **P. Tarakeshwar**, J. J. Palacios and D. M. Kim, Technical Proceedings of the IEEE Nanotechnology Materials and Devices Conference 2006, 566-567 (2006).

4. *Theoretical investigations of intermolecular interactions involving π-systems and their utility in the design of novel functional nanomaterials*, **P. Tarakeshwar** and K. S. Kim, Technical Proceedings of the 2003 Nanotechnology Conference and Trade Show, Vol. 3, 508-511 (2003).

PRESENTATIONS

Talks/Seminars -

1. Gave an invited seminar entitled "Intermolecular Interactions in Metal Electrode Interfaces and Hydrogen Storage Materials" in the Department of Chemistry, University of Pacific, Stockton, on October 2, 2007.
2. Gave an invited talk entitled "Intermolecular Interactions and their role in Understanding Metal-Molecule Contacts" in the Computational Chemistry Group of National Institute of Standards and Technology (NIST), Gaithersburg, on July 12, 2006.
3. Gave an invited seminar entitled "Computational Modeling and Designing of NanoElectronic Devices; Interface Chemistry in Molecular and CNT Transistors" in the Computational Science and Engineering Center, Samsung Advanced Institute of Technology, Yongin City, Korea on April 12, 2006.
4. Gave an invited seminar entitled "Quantum chemical investigations of metal-molecule contacts" in the Supercomputational Materials Simulation Laboratory, Korea Institute of Science and Technology, Seoul, Korea on April 30, 2004.
5. Gave an invited seminar entitled "A Computational Exploration of Intermolecular Interactions and Nanomaterial Design" in the School of Computational Sciences, Korea Institute of Advanced Study, Seoul, Korea on May 1, 2003.
6. Gave an invited seminar entitled "Molecular clusters of π systems: Relevance in molecular spectroscopy and the design of novel functional materials" as a part of the departmental colloquium series in the Department of Chemistry, University of Nevada, Las Vegas, on March 5, 2003.
7. Gave an invited seminar entitled "Molecular clusters of π systems: Versatile epitomes of molecular recognition and spectroscopy" in the Department of Chemistry, Utah State University, Logan, on March 4, 2003.
8. Gave an invited seminar entitled "Insights from theoretical investigations of intermolecular interactions involving π systems" in the Center for Complex Molecular Systems and Biomolecules, J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic on September 12, 2001.
9. Gave an invited seminar entitled "From molecular recognition to organic reaction mechanisms: A theoretical investigation of intermolecular interactions involving π systems" in the Institut für Chemie, Johann Wolfgang Goethe-Universität, Frankfurt, Germany on September 11, 2001.
10. Gave an invited seminar entitled "Theoretical investigations of intermolecular interactions: Bridging the gap between chemistry, physics and biology" as a part of the departmental colloquium series in the Department of Biological, Chemical, and Physical Sciences, Illinois Institute of Technology, Chicago, on March 21, 2001.

Meetings -

1. Gave an invited talk entitled “Unravelling the Vibrational Fingerprints of the Adenine-Thymine Base Pair”, at the 25th Austin Symposium on Molecular Structure and Dynamics in Dallas, on March 4, 2014.
2. Gave an invited talk entitled “Semiconducting Oxide Nanoparticle-Molecule Hybrids: Interfacial charge transfer and its implications in nanosensors, photo-catalysis, and solar-cells”, at the 24th Austin Symposium on Molecular Structure and Dynamics in Dallas, on March 6, 2012.
3. Gave an invited talk entitled “Hybrid molecule-metal oxide nano-particles: Interfacial charge transfer and its implications in sensors and solar cells”, at the “From Small to Large Molecular Systems: Challenges of Their Analysis” International Symposium held at Schloss Rauischholzhausen, Germany, on April 9, 2011.
4. Gave an oral presentation entitled “Hydrogen storage and catalytic properties of transition metal clusters: Bonding changes and saturation effects” at the 236th National meeting of the American Chemical Society held at Philadelphia during August 17-21, 2008.
5. Gave an invited talk entitled “Fostering Creativity and Innovation in Undergraduate Students: Curriculum vs. Pedagogy” at the “Innovative and Interdisciplinary Approaches to Science, Technology, & Mathematics Education: Future Outlook” symposium held at Seoul, Korea during June 20, 2008.
6. Gave an oral presentation entitled “Hydrogen Multicenter Bonds on Small Metal Clusters” at the 2008 APS March Meeting held at New Orleans, during March 10–14, 2008.
7. Gave an oral presentation entitled “Electrode-Molecule Interface Effects on Molecular Conductance” at the IEEE Nanotechnology Materials and Devices Conference 2006 (IEEE NMDC 2006) held at Gyeongju, Korea, during October 22-25, 2006.
8. Presented a poster entitled “Interface Study of Metal Electrode and Semiconducting Carbon Nanotubes: Effects of Electrode Atomic Species” at the IEEE Nanotechnology Materials and Devices Conference 2006 (IEEE NMDC 2006) held at Gyeongju, Korea, during October 22-25, 2006.
9. Gave an invited talk entitled “Characterization of Intermolecular Interactions Involving π Systems” at the “Intermolecular Interactions: New Challenges for ab initio Theory” workshop held at Telluride, Colorado during June 25 - July 2, 2006.
10. Presented a poster entitled “Modulation of the electronic structure of semiconducting nanotubes resulting from different metal contacts” at the "PACIFICHEM 2005” meeting held at Honolulu during December 15-20 2005.
11. Gave an oral presentation entitled “π-π Interactions. The Critical Role of Repulsive Energies” at the 230th National meeting of the American Chemical Society held at Washington D.C. during August 28-September 1, 2005.
12. Gave an oral presentation entitled “Characterization of Weak Intermolecular Interactions” at the Theory and Applications of Computational Chemistry (TACC-2004) conference held at Gyeongju, Korea, during February 15–20, 2004.
13. Presented a poster entitled “Theoretical investigations of intermolecular interactions involving π-Systems and their utility in the design of novel functional nanomaterials” at the 2003

Nanotechnology Conference and Trade Show, held at San Francisco, during February 23-27, 2003.

14. Gave an invited talk entitled "Molecular clusters of π systems: Relevance in molecular spectroscopy and the design of novel functional materials" in the 89th National Meeting of the Korean Chemical Society held at the Korean Military Academy, Seoul during April 20-21, 2002.

15. Gave an oral presentation entitled "Nature of π H-bonds: Insights from Theoretical Investigations of First-row Hydrides with Olefinic and Aromatic Systems" at the XIV Conference-Workshop on Horizons in Hydrogen Bond Research, held at Torino, Italy during September 2-7, 2001.

16. Presented a poster entitled "Theoretical investigations of the interaction of water clusters with π-systems: Role of cluster size and substituents"at the "PACIFICHEM 2000"meeting held at Honolulu during December 14-19, 2000.

17. Gave an oral presentation entitled "A Theoretical Investigation of the role of Lewis acid-Aromatic Substrate Complexes in Electrophilic Aromatic Substitution Reactions" at the 15th IUPAC meeting on Physical Organic Chemistry held at Goteborg, Sweden during July 8-13, 2000.

18. Presented a poster entitled "Theoretical investigations of the interaction of water clusters with π-systems: π vs. σ type of interaction" at the European Science Foundation meeting on "Molecules of Biological Interest in the Gas Phase" held at Les Houches, France during May 13-18, 2000.

19. Gave an oral presentation entitled "Lewis acids in electrophilic aromatic substitution reactions: An important role in activation of aromatic rings" at the 218th National meeting of the American Chemical Society held at New Orleans during August 22-26, 1999.

20. Presented a poster entitled "Aromatic π vs Olefinic π: A Theoretical Investigation of Interactions of first-row hydrides with Benzene / Ethylene" at the 5th World Congress of Theoretically Oriented Chemists (WATOC-99) held at London, UK, during August 1-6, 1999.

21. Presented a poster entitled "Activation of Aromatic Substrates in Electrophilic Aromatic Substitution Reactions: An Unusual Role of Lewis Acids" at the "34th Symposium of Theoretical Chemistry" held at Gwatt-Zentrum, Switzerland in September 1998.

22. Presented a poster entitled "An *ab initio* study of Ac-Asn-Pro-NMe" at the "IV National Bioorganic Symposium" held at BARC, Bombay in January 1992.

23. Presented a poster entitled "Molecular dynamic simulations of some of the repeat patterns of the circumsporozite protein of Plasmodium Falciparum" at the "National Conference on Mathematical Modeling" held at CCMB, Hyderabad in December 1991.

CONFERENCES/WORKSHOPS ORGANIZED

1. Was one of the co-organizers of a workshop entitled "Molecular and Nanoelectronics: Current Trends and Future Perspectives" held at the Korea Institute for Advanced Study, Seoul, Korea, during November 9-10, 2007.

2. Was one of the co-organizers of a lecture series entitled "KIAS Spring Lectures on Nanoelectronics", held at the Korea Institute for Advanced Study, Seoul, Korea, during April-May, 2006.

3. Was one of the co-organizers of a workshop entitled "Molecular and Nanoelectronics: Current Trends and Future Perspectives" held at the Korea Institute for Advanced Study, Seoul, Korea, during November 11-12, 2005.

4. Was the conference coordinator of "Theory and Applications of Computational Chemistry (TACC-2004)" conference held at Gyeongju, Korea, during February 15–20, 2004.

5. Was involved in the organization of "10th Korea-Japan Symposium of Theoretical and Computational Chemistry", held at Pohang, Korea, during January 12-15, 2003.

FUNDED PROJECT PROPOSALS

1. W. M. Keck Foundation, 07/1/2018-06/30/2021, From Carbon Chains to Pseudocarbynes: A New Class of Materials, A. K. Jones, P. R. Buseck, M. Meneghetti, **P. Tarakeshwar**, S. Sayres, and T. Steimle, Award Amount: $1,000,000

FELLOWSHIPS

Was a recipient of both the junior and senior research fellowships of the Council of Scientific and Industrial Research, New Delhi from Sep. 1988 to Aug. 1994.

MEMBERSHIPS

Life Member, World Association of Theoretical and Computational Chemists, WATOC (1998 -)

MISCELLANEOUS

Reviewer*:*

J. Am. Chem. Soc., ACS Appl. Mater. Interfaces, Langmuir, Nanoscale, Analyst, J. Photochem. Photobiol., J. Phys Chem., Phys. Chem. Chem. Phys., J. Comput. Chem., Chem. Phys., Sensors & Actuators: B., Chemical Biochimica et Biophysica Acta, Theoretical Chemistry Accounts, Science, Spectroscopy Letters, Spectrochim. Acta, Solid State Communications, etc.

Languages Known:

I have passed a one-year certificate course in German (1990) and French (1991).