Ashraf Ali

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● **EDUCATION**

1983, Ph.D., Chemistry, Indian Institute of Technology, Kanpur, India
1975, M.Sc., Physical Chemistry, University of Calcutta, India
1973, B.Sc., Honors in Chemistry, University of Calcutta, India

● **PROFESSIONAL POSITIONS**

NASA Goddard Space Flight Center (**GSFC**), Senior Scientist, Cassini-Huygens Project, 2006 – 2015
NASA GSFC, Principal Scientist, Astrochemistry Laboratory, Solar System Exploration Division,2003-2005
NASA GSFC, Principal Scientist, Astrochemistry Branch, Laboratory for Extraterrestrial Physics (**LEP**), 1995-2002; Senior Research Scientist, (LEP), 1991 – 1994
Research Scientist, Ames Laboratory, Department of Energy (**DOE**), Ames ,Iowa, 1990
Research Fellow, Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology (**CalTech**), Pasadena, California, 1987 – 1989
Research Associate, The Johns Hopkins University, Baltimore, Maryland, Chemistry, 1985-1987
Postdoctoral Fellow, School of Chemical Sciences, University of Illinois, Urbana, Illinois, 1983 – 1985

● **HONORS and AWARDS**

2008, Invited Visiting Professor, **CNRS**, Astrochimie Experimentale, I'Institut de Physique de Rennes, Rennes, FRANCE
2007, Invited Research Guest Investigator, Max Planck Institute for Astronomy, Heidelberg, GERMANY
2000, Sabbatical Leave Award (NASA GSFC), Pennsylvania State University, Chemistry, USA

● **RESEARCH PROFILE (Astrochemistry and Astrobiology)**

Stellar Evolutionary Process and the Origin of Life. Spectroscopy of Cold Molecules for Chemical Kinetics and Dynamics at Low Temperatures. Hypercoordinated Carbon (Three-Center Two-Electron Bonding) in Titan's Upper Atmosphere and its Astrobiological Consequences. Molecular Biology at the Nano Scale.

● **RESEARCH INTERESTS**

Radio Astronomy: Electromagnetic Interaction with Molecules, Antenna Coupled Quantum Limited Heterodyne Receiver Design and Millimeter Interferometry, Precision Spectroscopy and Metrology; Advanced Planetary Mass Spectrometry Electronic Engineering Techniques Development: The Optics of Charged Particles, Dynamics of Ion-Motion in an Ion-Trap Resonator between Two Electrostatic Mirrors, Atomic and Molecular Beam Methods; Quantum Optics and Nonlinear Processes.

● **COLLABORATORS and other AFFILIATIONS**

A.Canosa (Universite de Rennes1, France); A. W. Castleman, Jr. (Penn State University); B. Donn (NASA Goddard); H. D. Drew (University of Maryland, College Park); T. Henning (MPI, Germany); R. A. Marcus (California Institute of Technology); T. E. Murphy (UMD, College Park); H. B. Niemann (NASA Goddard); D. M. Neumark (University of California Berkeley); J. A. Nuth (NASA Goddard); G. A. Olah (University of Southern California); C. Puzzarini (University of Bologna, Italy); B. R. Rowe (Universite de Rennes1, France); E. C. Sittler, Jr. (NASA ,Goddard); P. F. Wahid (UCF, Florida); A. H. Zewail (California Institute of Technology).

● SYNERGISTIC ACTIVITIES

Laboratory measurements of molecular spectroscopy and quantum theoretical underpinnings toward planetary and astrophysical objects detection to disseminate the NASA Science Initiatives – the birth of our solar system and the origin of RNA-based life on Earth through participation and numerous presentations at National and International Conferences, Laboratories and Universities. Reviewer of NASA Projects and Peer-Review International Scientific Journals in related fields. The CAPS (Cassini Plasma Spectrometer) and INMS (Ion Neutral Mass Spectrometer) Cassini-Huygens Lead Science Investigator at NASA Goddard (2010 – 2015). The CAPS and INMS related Science on the relevance and significance of extraterrestrial abiological organic synthesis was carried out in a joint collaboration with Professor Cristina Puzzarini at the Dipartmento di Chimica “Giacomo Ciamician”, Universita di Bologna, Bologna, Italy (https://site.unibo.it/rotational-computational-spectroscopy/en);
Website: http://star.sns.it/

● STATEMENT of RESEARCH

The Cassini-Huygens mission led by **NASA** to Saturn system was the largest and the most ambitious effort in the exploration of planetary science. The observation of the chemistry of hypercoordinated carbon on Titan by the instruments onboard the Cassini spacecraft is a major breakthrough and by far the largest “surprise” in terms of planetary chemistry in our solar system. It provides a direct hint at how the molecular building blocks of life (e.g. the sugars and the nucleobases in RNA-first world) on Earth originated under prebiotically plausible conditions, since the creation of the first cosmological objects.

● REPRESENTATIVE PUBLICATIONS

2019 Extraterrestrial Abiological Synthesis of Organics in Space and its Significance to Chemical Evolution and the Origin of Life, A. Ali. Phys. Life Rev. https://doi.org/10.1016/j.plrev.2019.08.010

2017 Spectroscopic Characterization of Key Aromatic and Heterocyclic Molecules: A Route toward the Origin of Life, C. Puzzarini, A. Baiardi, J. Bloino, V. Barone, T. E. Murphy, H. D. Drew, A. Ali. Astron. J. 154: 82 (10pp).

2015 Organic Chemistry in Titan’s Upper Atmosphere and its Astrobiological Consequences: I. Views Towards Cassini Plasma Spectrometer (CAPS) and Ion Neutral Mass Spectrometer (INMS) Experiments in Space, A. Ali, E. C. Sittler Jr., D. Chornay, B.R. Rowe, C. Puzzarini. Planet. Space Sci. 109 – 110, 46.

2014 Accurate Spectroscopic Characterization of Protonated Oxirane: A Potential Prebiotic Species in Titan’s Atmosphere, C. Puzzarini, A. Ali, M. Biczysko, V. Barone. Astrophys. J. 792:118 (6pp).

2013 Cyclopropenyl Cation – the Simplest Huckel’s Aromatic Molecule – and its Cyclic Methyl Derivatives in Titan’s Upper Atmosphere, A. Ali, E. C. Sittler, D. Chornay, B. R. Rowe, C. Puzzarini.

Planet. Space Sci. 87, 96.

2007 The Oxygen Isotope Effect in the Earliest Processed Solids in the Solar System: Is it a Chemical Mass – Independent Process, A. Ali, J. A. Nuth. Astron. Astrophys. 467, 919.

2006 Silicon Oxide Nanoparticles Reveal the Origin of Silicate Grains in Circumstellar Environments, A.C.Reber, P. A. Clayborne, J. U. Reveles, S. N. Khanna, A. W. Castleman, Jr., A. Ali. Nano Lett. 6, 1190.

Biographical Sketches:

I was born in Calcutta, India in 1953, 5th November. I obtained both Bachelor and Master of Science from University of Calcutta in 1973 and 1975 respectively, majoring in Chemistry. In early 1983, I received Ph.D. in Chemical Physics from Indian Institute of Technology, Kanpur, India under the supervision of Professor P. K. Ghosh, who is well respected an experimental Chemical Physicist in India and abroad. My long interests in electronic engineering techniques development are the result of reflection on the mentor Professor P. K. Ghosh, who first introduced me during the period of my Ph.D. thesis laboratory plasma instrumentation with emphasis on Mass Spectrometry Optics of Charged Particles trapping in an inhomogeneous three dimensional radio frequency quadrupole field.

After my Ph.D. thesis I then headed to the School of Chemical Sciences at the University of Illinois, Urbana, Illinois to work with Professor James M. Lisy as a postdoctoral fellow (1983 – 1985). My research involved infrared spectroscopy of weakly bound van der Waals Complexes and the study of intermolecular forces using supersonic molecular beams. It is a field of fundamental importance for most of molecular biology at the Nano-Scale. The detection of microwave rotational transitions in weakly bonded molecules in the chemistry of interstellar space will play a critical impact on the field of Astrobiology – a subject about which there has been considerable speculation, yet without arriving at a certain identification that leads verifiable conclusions.

I spent 1985 – 1987 as Research Associate at the Department of Chemistry, The Johns Hopkins University, Baltimore, Maryland and 1987 – 1989 as Research Fellow at Arthur Amos Noyes Laboratory of Chemical Physics, Caltech (California Institute of Technology), Pasadena, California. With Professor Paul J Dagdigian at the Johns Hopkins University, I studied State-to-State Collisional Interelectronic and Intraelectronic Energy Transfer between Rotational Levels of Diatomic Molecules and Free Radicals by Optical-Optical Double Resonance Technique using home-built Pulsed Dye Lasers. I pursued 1987-1989 in the laboratory of late Professor Aron Kuppermann at Caltech the Art of Designing Crossed Molecular Beam Apparatus. There I first got encountered and introduced myself with late Professor Ahmed H. Zewail, 1999 Nobel laureate in Chemistry. He taught me Molecular Quantum Electronics and the subject "COHERENCE" in Physics, those left a lasting impression on the approach of my research – observing the chemical evolution of the Universe. I have found Ahmed obsessed through the rest of his life with the idea of bringing in Chemistry the concept of Quantum Coherence in Physics.

After a brief stay 1990 as a Research Scientist at Ames Laboratory, Department of Energy, Ames, Iowa, I moved to National Aeronautics and Space Administration (NASA) as a Senior Scientist at the Goddard Space Flight Center (GSFC) Laboratory for Extraterrestrial Physics (LEP), Astrochemistry Division, Greenbelt, Maryland. Nearly thirty years ago, I moved from the spectroscopy and chemical dynamics field to the astrochemistry field, and this was largely triggered by a fundamental question of our ability of observing the molecule-solid phase transition and the synthesis of nanoparticles in stellar outflows by millimeter-wave astronomy and angular resolved radio interferometric techniques. Measuring the mass loss regulating post main-sequence stellar evolution and how are molecules in the interstellar medium (ISM) incorporated into the new generation stars and planets providing a potential island for life are of considerable interest toward a comprehensive understanding of the history of the Universe. Stellar systems are formed through the collapse of molecular clouds, which in turn in their lifetimes return copious amounts of atomic and molecular material enriched by nucleosynthesis to the ISM. An in-depth understanding of this cyclic interaction between the stars and the interstellar medium in galaxies is the heart of astrochemistry. With Coherent Detection systems we can observe this process through detecting molecular rotational line transitions and fine-structure transitions of atoms, ions and isotopes as the cool ISM reprocesses during its lifecycle essentially all central source radiation to the Far Infrared (FIR) and sub-mm regime and give clear indications of its composition and physical conditions.

Providing the concept, definition and development of laboratory and space instruments, I became the Lead Research Investigator at the Goddard Space Flight Center (GSFC) 1990 -2015 toward planetary and astrophysical detection and the exploration of chemistry of planets in our solar system and the origin of RNA-based life on Earth (Biology at the Nano Scale). During this period from 1991 to 2015, I maintained a long standing collaboration with Senior Faculty Members from various Universities and National Laboratories at US and abroad.

During the period from 1991 to 2005, my research group was involved in the area of Solid State Astronomy toward a comprehensive understanding of grain formation and the mechanisms of mass loss in circumstellar shells of AGB stars and the gas/dust ISM replenishment. To investigate a question of the composition of silicates in circumstellar shells of evolved stars in the interstellar medium, the research involved the formation of molecular clusters of Silicon Monoxide using the technique of Laser Ablation and Pulsed Cluster Beam Method, and Femtosecond Laser Photoionization Time-of-Flight Mass Spectrometry. The most significant result of the experiment is the proposed geometry of large clusters of Silicon Monoxide. The architecture of the Silicon Monoxide large clusters is unique with a core of Si atoms and a shell of SiO_2 molecules. Recent infrared spectroscopic studies of cations of small clusters of silicon monoxide molecule in ion trap confirm the presence of Si-Si bond (Garand et.al., Phys. Chem. Chem. Phys. 10, 1502 (2008). Rotational spectroscopic studies in cluster beams and/or in ion traps are critical to allow astronomical interferometric spatial observations to bear on the fascinating problem of composition of silicates in the circumstellar shells of evolved stars in the interstellar medium in a novel geometry with a core of Si atoms and a shell of SiO2 molecules. It was a long collaborative research effort between my research group consisting of late Dr. Bertram Donn, Dr. Joseph A. Nuth and myself at the NASA Goddard Space Flight Center, and the research group of late Professor A. W. Castleman, JR. at the Pennsylvania State University.

Following systematic astronomical observations of interstellar matter, especially in the infrared and far-infrared spectrum including millimeter interferometry, interest had been grown to identify the chemical and isotopic composition of interstellar solids and understanding the molecule-solid multicomponent phase transition process existing in the Universe. This scientific approach indeed made advances to the discovering the birth of our solar system and the origin of solid matter that constitutes planetary system of our own. The discovery of covariation of $^{17}O/^{16}O$ and $^{18}O/^{16}O$ isotopes ratios in refractory mineral oxides in the earliest processed solids in the solar system with an equal fractionation, despite the difference in mass, was a great turning point in cosmochemistry studies. The origin of mass-independent anomalies in oxygen isotopes fractionation is not nucleosynthetic. The effect is caused by the molecular symmetry induced stabilization of an activated non-symmetric trimer (e.g. $^{16}OSi^{18}O$) during a high-temperature reaction at the gas-surface interface of a growing solid grain such as silicates:

$$SiO(ads) + O(ads) = SiO_2^*(ads) \rightarrow SiO_2(g).$$

The ads above stands for adsorption on the surface. Because of its large ro-vibrational density of states an asymmetric trimer molecule is preferentially stabilized over the one that is symmetric ($^{16}OSi^{16}O$) in the bimolecular association reaction in the gas phase. The surface analog of microcanonical transition state theory is brought here. The importance of mass-independent anomalies in oxygen isotopes in the earliest processed inorganic solids in the solar system is well reflected in the recent contributions by Professor R. A. Marcus (Nobel Laureate in Chemistry in 1992) at the California Institute of Technology. Details can be seen in our recent publication (Astron. Astrophys. 467, 919, 2007) and references therein. The unimolecular dissociation rate of an activated ro-vibrational trimer molecule in the microcanonical RRKM transition state theory is molecular symmetry induced, and this step plays a pivotal role in the mechanistic interpretation of the origin of earliest processed inorganic solids in the solar system.

Subsequently in the year 2005, I moved as one of the Lead Program Scientists in the Cassini-Huygens Project at NASA Goddard Space Flight Center (GSFC). In the exploration of planetary science the Cassini – Huygens mission led by NASA to Saturn System was the most ambitious effort. The observation of abiological synthesis of hydrocarbons, their derivatives and ions (Carbocations and Carbanions) on Titan by Quadrupole Mass Spectrometer (QMS) and Electrostatic Analyzer (ESA) instruments onboard the Cassini spacecraft is a major breakthrough, and by far the largest "surprise" in terms of chemistry of planets in our solar system. This project was carried out by a long term collaborative research effort between my research group at GSFC and the research group of my colleague Professor Cristina Puzzarini at the Departmento di Chimica "Giacomo Ciamician" , University of Bologna, Italy (https://site.unibo.it/rotational-computational-spectroscopy/en). The organic synthesis on an abiotic body Titan in our solar system proceeds through the conversion of most abundant methane to methonium ion CH_5^+ and Olah's related nonclassical carbonium ion chemistry. A nonclassical Two-Electron Three-Carbon-Center (2e, 3c) bound penta- or tetracoordinated carbonium ion structure is found to play a dominant role on the extraterrestrial abiological hydrocarbon chemistry. The Cassini observation of the beginning of biological synthesis in our solar system thus surprisingly points that the chemistry of carbon with unusual valence and the nature of chemical bond is of equal importance with the Lewis concept of two-electron two-center covalent bond. No one has stated this more boldly than the chemistry Nobel Laureate George Andrew Olah : "Of particular interest to us is the remarkable detection of varied carbocations and their similarity with their terrestrial analogues. The proven similarity with our terrestrial studied chemistry provides the first scientific evidence that our Earth is not a unique celestial body for producing the chemical building blocks".

Young Planetary Systems are formed from the hard vacuum of interstellar space, in a vast cosmos, over approximately ten exponent seven years. In two most recent landmark papers Professor George Andrew Olah (1994 Nobel Laureate in Chemistry) and a number of co-authors stated that chemistry of carbon for life's origin and subsequent biological cell transformation during this interstellar evolutionary process is also intricately linked to this surprising abiolgical chemistry of synthesis organics on Titan observed (J. Amer. Chem. Soc. 138,1717,2016; ibid., 138,6905,2016). It is a most impressive extension of our published research by the late Professor George Andrew Olah who was one of the legends in Chemistry in the twentieth century and early twenty-first. Both Methane and Methanol (monooxygenated Methane) are shown in these perspectives to be the key Molecular SYNTHON of biological cell evolution and life's origin. The merit for understanding the initial stage of life's origin and subsequent biological transformation to cells goes to Astrophysical Observers, Planetary Astronomers, Modern pioneering Studies in Biological Sciences, including thousands of researchers who were directly or indirectly involved for decades in the NASA Cassini-Huygens Mission development project. In essence, our perspectives are the ICONIC representation of studies made possible by those researchers.

A comprehensive spectroscopic view and understanding is required of how interstellar matter is evolved and brought into stars and planets. This is ultimately related to the understanding of the birth of our own solar system and the origin of Life on Earth (and elsewhere ?). The coherent heterodyne detection systems with angle-resolved interferometry are needed for spectral and spatial resolutions observations in the far-infrared (FIR) and sub-millimeter window. The frequency resolution on the order of ~ 100 KHz spectroscopy allows one to probe the chemical processes in diverse astronomical objects such as in diffuse clouds, dense quiescent molecular clouds, star forming regions, and protoplanetary disks. The physical basis for the interactions between matter and radiation in the THz , laboratory measurements and theoretical underpinnings of molecular rotational spectroscopy are the integral part of my current research group in Astrochemistry toward accomplishing of an important task of a millimeter/sub-millimeter-wave heterodyne mixer based receiver development with engineering challenges. The design concepts and development of antenna coupled heterodyne sensor together with laboratory measurements and quantum mechanical theoretical underpinnings of molecular rotational spectroscopy will be carried out in the Department of Physics at the University of Maryland, College Park. Over the next decade and beyond, we expect to undertake research that will explore “Cosmic Origins Theme” – how galaxies, stars, planets, and cosmic structure come into being and when and how the elements of life in the Universe arose.