Metallofullerene

Metallofullerene
Dear Colleagues,

In the last issue of AstroPAH, the Picture of the Month was a beautiful image of a large scale PAH outflow in the M82 galaxy. To start our new year with fireworks, a supernova explosion was detected in this galaxy last January (http://apod.nasa.gov/apod/ap140124.html).

To complete this wonderful start of the year, we interviewed Christine Joblin for our In Focus section.

Don’t miss any of the abstracts this month – we have works from molecular to galactic scales – and the announcement of the Second Annual LAD Meeting.

Publish the abstracts of your papers or thesis and advertise scientific meetings in AstroPAH. It is subscribed by more than 150 researchers interested in the Astronomical PAHs field.

You may send contributions to AstroPAH any time. The deadline for contributions to appear in the next issue is the 7th of March 2014. The next issue of AstroPAH will be out on the 18th of March 2014.

For more information on AstroPAH, visit our website:

http://astropah-news.strw.leidenuniv.nl.

Best regards

The Editorial Team
PAH Picture of the Month

Metallofullerenes like Na@C$_{60}$ can be created in oxygen and hydrogen rich environments under highly energetic conditions, such as in supernova ejecta. The picture in the cover shows the FT-ICR mass spectrum of cluster cations that spontaneously form in condensing carbon vapor seeded with Na (10 psi He gas flow, $\sim$35 mJ cm$^{-2}$ fluence). (Insets) Na@C$_{60}$ clearly resolved from empty C$_{62}$ and the relative abundance of Na@C$_{2n}$ species. See the Abstract section for more details. Credits: P. W. Dunk.
Dr. Christine Joblin, is a research scientist at the Institut de Recherche en Astrophysique et Planétologie (IRAP) in Toulouse, France. Her research focuses on the physics and chemistry of interstellar dust and molecules with a special interest in polycyclic aromatic hydrocarbons (PAHs). To address this subject, she uses an approach combining astronomical observations and laboratory studies. She is also collaborating with physicists and chemists, especially in the field of quantum chemistry. She has developed the PIRENEA setup, which is devoted to the study of the photophysics and chemistry of PAHs and related species in conditions that approach those found in interstellar space. She is also participating in astronomical observations, using both space observatories (ISO, Spitzer, Herschel) and ground-based telescopes (IRAM,...), mainly in the IR and mm ranges. Her main interest is in the spectro-imagery of photodissociation regions to study the evolution of very small dust particles and their role in chemistry, in particular in the formation of H₂. Here is her interview for AstroPAH!

**Prelude**

I was asked for this interview because I am a woman with 25 years of experience in the astroPAH field and there are not so many candidates. Fortunately, the situation is changing. Just have a look at the editorial board of the AstroPAH newsletter! Still my younger colleagues would like to know more on how I came to the astroPAH field and how I managed to combine my busy scientific life with my personal life. I tried to answer in a very honest way.

**My advice to the young generation**

There is not a single way in this life. Some of us have more opportunities to make choices. You have to catch yours and, maybe more importantly, you have to understand why you made these choices. That will give you enough resources to go through the stormy phases of life; not everything is going to be easy, not everything is going to be according to plan. A scientist is for me like an artist. He/she comes to science because he/she is looking for something more than a job.
Why study interstellar PAHs?

From my first steps in science, I worked in the field of interstellar PAHs and I still find it completely fulfilling. This is not because the topic is about interstellar PAHs; in fact I know some colleagues who would tell me "All this may be complete fantasy, and what if they do not exist?" I am not afraid at all of this possibility since all the work that has been triggered by the PAH hypothesis remains of great interest. From the methodological point of view, the interplay between laboratory experiments/simulations, observations of natural environments, and modelling is the way to progress in various fields. If tomorrow I was asked to contribute to a project in another field that uses a similar approach, for instance environmental chemistry, I feel I could do it. In addition, from the very beginning, the AstroPAH field is very interdisciplinary in nature involving astrophysicists, physicists and chemists. PAHs are fun species, simple enough from a chemical point of view that a physicist like me can pretend studying them. They are macromolecular species at the frontier of the nanoworld and tackling their fundamental properties can have impact in many fields. Finally, PAHs are not exotic species; they are easy to produce and are unfortunately a major pollutant in our everyday life. Understanding their chemical properties can also lead to a better control of their production.

How I came to the field and built my professional and personal life:

I studied astrophysics in my second year of Master's degree. I was fascinated by a course on the interstellar medium and I asked the Professor, Pierre Léna, to guide me in the selection of research topics. He told me that there was a new and promising subject related to the proposal that large polycyclic aromatic hydrocarbons (PAHs) are abundant species in the interstellar medium. Following his advice, I performed my Master's training in 1989 in the group of Alain Léger, one of the two leading groups in the subject of interstellar PAHs. The group was conducting experiments at the synchrotron Super-Aco in Orsay to measure the vacuum-UV absorption cross-sections of PAHs and determine their contribution to the interstellar UV curve. I hesitated to continue in the same group (Alain Léger and Louis d'Hendecourt) for my PhD project since I was also tempted to join Pierre Boissel to build an ion trap dedicated to the study of the photophysics and chemistry of PAHs in interstellar conditions. However, I received advices that this may be too risky in the timeline of a PhD project. In addition, Alain Léger ended with the attractive proposal of sending me to Hawaii to perform observations at the CFH Telescope. This made my decision! The observations led to the detection of two diffuse interstellar bands (DIBs) in the near-infrared and a paper in Nature that was published on the day of my 23rd birthday. My PhD experience was very rich and a lot of new results came out. In addition to the UV measurements, we developed a high temperature oven to record the evolution of the IR spectra of PAHs with temperature. These results are still of use today to quantify anharmonic effects that have to be taken into account while modelling the infrared emission of hot PAHs.

As a post-doctoral fellow, I naturally joined the group of Lou Allamandola at NASA Ames, the other leading group in the study of interstellar PAHs. After having worked on gas-phase PAHs, I discovered the world of rare-gas matrices, working with Farid Salama on the electronic spectroscopy of PAH cations and the connection with DIBs. I worked more specifically on the emission of PAH cations, having in mind that some DIBs are observed in emission. I had my first talk at the DIB conference in Boulder in 1994 and reported evidence for visible luminescence of
PAHs. I was very anxious and I remember that Lou was supporting me as he would do during a baseball game, "Christine, go for it!" Unfortunately I was not so successful. John Maier, one of the biggest experts in the field, strongly argued at the end of my presentation that it is well known that PAH cations do not fluoresce. We published the fluorescence spectrum of the perylene cation and this result has now been rationalized by the work of quantum chemists. We still have a lot to learn on this subject and I am glad my colleagues in Lyon (Serge Martin’s team) recently involved me in their study of the cooling of PAH cations in storage rings. Under the beautiful sky of California or at the cappuccino machine (I cannot remember) I also met Xander Tielens who involved me in infrared observations and their analysis, which I appreciated a lot since years taught me that I am not the kind of person who can focus on a single question/project. Finally, I met there two very important people in my life, Irina who became my best friend and is now Professor at the Georgia Institute of Technology in Atlanta, and my future husband, Professor in physics at the University of Toulouse, who still helps me combine my busy scientific life with my mother’s life.

When I obtained my CNRS permanent position in Toulouse in 1995 I had two big projects: develop an original setup for laboratory astrophysics made of a cold ion trap to study PAHs in cosmic environment, and raise a family.

The PIRENEA project was challenging from the beginning. Laboratory astrophysics was a new activity at CESR (Centre d’Etude Spatiale des Rayonnements, now IRAP) in Toulouse, where mainly instruments for space missions were developed. Because the setup was requiring an intense magnetic field, the laboratory was moved from the main building to the house that was initially planned for the concierge, with several drawbacks in particular a limited area and a poor thermal isolation killing the stability of the lasers. A few years after my arrival, we sadly lost our group leader, Guy Serra, who was really supporting this new activity. I obtained the technical support from one engineer, Michel Armengaud, coming from the plasma physics community and for years we courageously designed and built this complex experiment. I had to write so many proposals to obtain step by step the necessary financial supports. I had difficulties to attract PhD students in the laboratory since most of them were more interested in astronomical observations and/or modelling. In total three PhD students (all female students) and very recently one post-doctoral fellow contributed to the setup. PIRENEA is mainly homemade and it took a long time to develop and optimise it, including several interfaces to study the photophysics and chemistry of cold isolated PAH ions or related species. Certainly not enough of the obtained results are published yet but that will come. We have built a real expertise around this activity, which gathers today a small team of innovative engineers and young talented researchers. I am very fortunate to collaborate with very good physicists and chemists, amongst whom Giacomo Mulas (Cagliari Observatory), Fernand Spiegelman (University of Toulouse), Stephan Schlemmer (University of Cologne), Paul Mayer (University of Ottawa) and their teams. I have to acknowledge also very fruitful interactions with astroph ysicists, in particular Maryvonne Gérin at the École Normale Supérieure (ENS) in Paris. Finally, I was lucky to be supported all these years by Dominique Le Quéau, starting the day I knocked on his door at the ENS-Paris in July 1987. He was the director of my Institute when I entered CNRS and he strongly supported the development of the PIRENEA setup. Today he is still active in supporting our activity through a collaborative project with the dusty plasma community. I am so grateful to him for providing me with many opportunities to be creative in my work.

The AstroPAH field constitutes my main scientific activity but not the only one. I also try to
be helpful by taking charge of collective responsibilities. In addition, I do not forget that I have two wonderful teenagers at home. They know they have a mother who is dedicated to her work. Since a day is only 24 hours, it can happen that I come back at home full of electricity and get exposed to a glare from the father since it is getting late. In these moments, I cannot wave a magic wand but I found that being creative in the kitchen is quite easy for me and makes all family much happier in front of healthy food. I also make sure I listen to my kids when they call for a particular attention.

The future

After many years of studying the chemical and physical properties of PAHs and trying to understand the astrophysical media in which they are observed, mainly the photodissociation regions, one of the new opportunities in the coming years will be to tackle the big question of PAH formation, in particular in the environments of evolved stars. Only a few groups have worked on this question so far and there is a lot to explore to identify the key processes that lead to the formation of PAHs and interstellar dust in general. The Nanocosmos project will address this question using a multidisciplinary approach. It will start soon with a grant of the European Research Council to support the synergy between the views of three PIs: Jose Cernicharo and Jose A. Martín Gago in Madrid and myself in Toulouse. I hope that this project will contribute to make the AstroPAH field even more attractive for the young generation and give them opportunities to obtain the positions in science they wish for.
Recent Papers

Andromeda’s Dust

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Spitzer Space Telescope and Herschel Space Observatory imaging of M31 is used, with a physical dust model, to construct maps of dust surface density, dust-to-gas ratio, starlight heating intensity, and polycyclic aromatic hydrocarbon (PAH) abundance, out to $R \approx 25$ kpc. The global dust mass is $M_\text{d} = 5.4 \times 10^7 M_\odot$, the global dust/H mass ratio is $M_\text{d}/M_\text{H} = 0.0081$, and the global PAH abundance is $\langle q_{\text{PAH}} \rangle = 0.039$. The dust surface density has an inner ring at $R = 5.6$ kpc, a maximum at $R = 11.2$ kpc, and an outer ring at $R \approx 15.1$ kpc. The dust/gas ratio varies from $M_\text{d}/M_\text{H} \approx 0.026$ at the center to $\sim 0.0027$ at $R \approx 25$ kpc. From the dust/gas ratio, we estimate the interstellar medium metallicity to vary by a factor $\sim 10$, from $Z/Z_\odot \approx 3$ at $R = 0$ to $\sim 0.3$ at $R = 25$ kpc. The dust heating rate parameter $\langle U \rangle$ peaks at the center, with $\langle U \rangle \approx 35$, declining to $\langle U \rangle \approx 0.25$ at $R + 20$ kpc. Within the central kiloparsec, the starlight heating intensity inferred from the dust modeling is close to what is estimated from the stars in the bulge. The PAH abundance reaches a peak $q_{\text{PAH}} \approx 0.045$ at $R \approx 11.2$ kpc. When allowance is made for the different spectrum of the bulge stars, $q_{\text{PAH}}$ for the dust in the central kiloparsec is similar to the overall value of $q_{\text{PAH}}$ in the disk. The silicate-graphite-PAH dust model used here is generally able to reproduce the observed dust spectral energy distribution across M31, but overpredicts 500 $\mu$m emission at $R \approx 2-6$ kpc, suggesting that at $R = 2-6$ kpc, the dust opacity varies more steeply with frequency (with $\beta \approx 2.3$ between 200 and 600 $\mu$m) than in the model.

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http://iopscience.iop.org/0004-637X/780/2/172/
Quadrupole ion trap/time-of-flight photo-fragmentation spectrometry of the hexa-peri-hexabenzocoronene (HBC) cation

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We have studied the photo-fragmentation of the HBC cation \( \text{C}_{42}\text{H}_{18}^+ \), a large PAH cation of potential astrophysical interest. HBC cation photo-fragment patterns are measured upon irradiation by an unfocused Nd:YAG laser (532 nm) for different experimental conditions, using quadrupole ion trap, time-of-flight mass spectrometry. Both stepwise dehydrogenation of \( \text{C}_{42}\text{H}_{18}^+ \) and \( \text{C}_2/\text{C}_2\text{H}_2 \) loss pathways are identified as relevant photodissociation routes.

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Concavity Effects on the Optical Properties of Aromatic Hydrocarbons

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We study the modifications on the ground and excited state properties of polycyclic aromatic hydrocarbons (PAHs), induced by the variation of concavity and \( \pi \)-connectivity. Inspired by experimentally feasible systems, we study three series of PAHs, from H-saturated graphene flakes to geodesic buckybowls, related to the formation of fullerene \( \text{C}_{60} \) and \( \text{C}_{50} \)-carbon nanotube caps. Working within the framework of quantum chemistry semi-empirical methods AM1 and ZINDO/S, we find that the interplay between concavity and \( \pi \)-connectivity shifts the bright optical lines to higher energies, and introduces symmetry-forbidden dark excitations at low energy. A generally good agreement with the available experimental data supports our results, which can be viewed as the basis for designing optical properties of novel curved aromatic molecules.

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A mid-IR comparative analysis of the Seyfert galaxies NGC 7213 and NGC 1386

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New Gemini mid-infrared spectroscopic observations together with Spitzer Space telescope archival data, are used to study the properties of the dusty torus and circumnuclear star formation in the active galaxies NGC 7213 and NGC 1386. Our main conclusions can be summarised as follows. Polycyclic aromatic hydrocarbon (PAH) emission is absent in the T-ReCS nuclear spectra but is ubiquitous in the data from Spitzer at distances above 100 pc. Star formation rates surface densities are estimated from the 12.8μm [NeII] line strengths leading to values close to 0.1 M⊙ yr⁻¹ kpc⁻². Analogous estimates based on photometric fluxes of IRAC’s 8 μm images are higher by a factor of almost 15, which could be linked to excitation of PAH molecules by older stellar populations. T-ReCS high spatial resolution data reveal silicate absorption at λ9.7μm in the central tens of parsecs of the Seyfert 2 NGC 1386, and silicate emission in the Seyfert 1 galaxy NGC 7213. In the case of NGC 1386 this feature is confined to the inner 20 pc, implying that the silicate might be linked to the putative dusty torus. Finally, by fitting CLUMPY models to the T-ReCS nuclear spectra we estimate the torus physical properties for both galaxies, finding line of sight inclinations consistent with the AGN unified model.

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Metallofullerene and fullerene formation from condensing carbon gas under conditions of stellar outflows and implication to stardust

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Carbonaceous presolar grains of supernovae origin have long been isolated and are de-
termined to be the carrier of anomalous $^{22}$Ne in ancient meteorites. That exotic $^{22}$Ne is, in fact, the decay isotope of relatively short-lived $^{22}$Na formed by explosive nucleosynthesis, and therefore, a selective and rapid Na physical trapping mechanism must take place during carbon condensation in supernova ejecta. Elucidation of the processes that trap Na and produce large carbon molecules should yield insight into carbon stardust enrichment and formation. Herein, we demonstrate that Na effectively nucleates formation of Na@C$_{60}$ and other metallofullerenes during carbon condensation under highly energetic conditions in oxygen- and hydrogen-rich environments. Thus, fundamental carbon chemistry that leads to trapping of Na is revealed, and should be directly applicable to gas-phase chemistry involving stellar environments, such as supernova ejecta. The results indicate that, in addition to empty fullerenes, metallofullerenes should be constituents of stellar/circumstellar and interstellar space. In addition, gas-phase reactions of fullerenes with polycyclic aromatic hydrocarbons are investigated to probe "build-up" and formation of carbon stardust, and provide insight into fullerene astrochemistry.

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**Spitzer Space Telescope** spectra of post-AGB stars in the Large Magellanic Cloud —polycyclic aromatic hydrocarbons at low metallicities

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This paper reports variations of polycyclic aromatic hydrocarbons (PAHs) features that were found in Spitzer Space Telescope spectra of carbon-rich post-asymptotic giant branch (post-AGB) stars in the Large Magellanic Cloud (LMC). The paper consists of two parts. The first part describes our Spitzer spectral observing programme of 24 stars including post-AGB candidates. into post-AGB stars, AGB stars, planetary nebulae and other types. The latter half of this paper presents the analysis of PAH features in 20 carbon-rich post-AGB stars in the LMC, assembled from the Spitzer archive as well as from our own programme. We found that five post-AGB stars showed a broad feature with a peak at 7.7 \( \mu \text{m} \), that had not been classified before. Further, the 10–13 \( \mu \text{m} \) PAH spectra were classified into four classes, one of which has three broad peaks at 11.3, 12.3 and 13.3 \( \mu \text{m} \) rather than two distinct sharp peaks at 11.3 and 12.7 \( \mu \text{m} \), as commonly found in HII regions. Our studies suggest that PAHs are gradually processed while the central stars evolve from post-AGB phase to PNe, changing their composition before PAHs are incorporated into the interstellar medium. Although some metallicity dependence of PAH spectra exists, the evolutionary state of an object is more significant than its metallicity in determining the spectral characteristics of PAHs for LMC and Galactic post-AGB stars.

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Polycyclic aromatic hydrocarbon ionization as a tracer of gas flows through protoplanetary disk gaps

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Planet-forming disks of gas and dust around young stars contain polycyclic aromatic hydrocarbons (PAHs). We aim to characterize how the charge state of PAHs can be used as a probe of flows of gas through protoplanetary gaps. In this context, our goal is to understand the PAH spectra of four transitional disks. In addition, we want to explain the observed correlation between PAH ionization (traced by the 6.2/11.3 feature ratio) and the disk mass (traced by the 1.3 mm luminosity). We implement a model to calculate the charge state of PAHs in the radiative transfer code MCMax. The emission spectra and ionization balance are calculated. A benchmark modeling grid is presented that shows how PAH ionization and luminosity behave as a function of star and disk properties. The PAH ionization is most sensitive to ultraviolet (UV) radiation and the electron density. In optically thick disks, where the UV field is low and the electron density is high, PAHs are predominantly neutral. Ionized PAHs trace low-density optically thin disk regions where the UV field is high and the electron density is low. Such regions are characteristic of gas flows through the gaps of transitional disks. We demonstrate that fitting the PAH spectra of four transitional disks requires a contribution of ionized PAHs in gas flows through the gap. The PAH spectra of transitional disks can be understood as superpositions of neutral and ionized PAHs. For HD97048, neutral PAHs in the optically thick disk dominate the spectrum. In the cases of HD169142, HD135344B and Oph IRS 48, small amounts of ionized PAHs located in the gas flows through the gap are strong contributors to the total PAH luminosity. The observed trend between the disk mass and PAH ionization may imply that lower-mass
disks have larger gaps. Ionized PAHs in gas flows through these gaps contribute strongly to their spectra.

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Formation history of polycyclic aromatic hydrocarbons in galaxies

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Polycyclic aromatic hydrocarbons (PAHs) are some of the major dust components in the interstellar medium (ISM). We present our evolution models for the abundance of PAHs in the ISM on a galaxy-evolution timescale. We consider shattering of carbonaceous dust grains in interstellar turbulence as the formation mechanism of PAHs while the PAH abundance can be reduced by coagulation onto dust grains, destruction by supernova shocks, and incorporation into stars. We implement these processes in a one-zone chemical evolution model to obtain the evolution of the PAH abundance in a galaxy. We find that PAH formation becomes accelerated above certain metallicity where shattering becomes efficient. For PAH destruction, while supernova shock is the primary mechanism in the metal-poor environment, coagulation is dominant in the metal-rich environment. We compare the evolution of the PAH abundances in our models with observed abundances in galaxies with a wide metallicity range. Our models reproduce both the paucity of PAH detection in low metallicity galaxies and the metallicity-dependence of the PAH abundance in high-metallicity galaxies. The strong metallicity dependence of PAH abundance appears as a result of the strong metallicity dependence of the dust mass increase by the accretion of metals onto dust grains, which are eventually shattered into PAHs. We conclude that the observational trend of the PAH abundance can be a natural consequence of shattering of carbonaceous grains being the source of PAHs. To establish our scenario of PAH formation, observational evidence of PAH formation by shattering would be crucial.

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Second Annual Laboratory Astrophysics Division Meeting

http://aas.org/meetings/aas224/lad

The second LAD meeting devoted to the interplay between laboratory astrophysics and other fields in astronomy, planetary science and related sciences will be held jointly with the 224th Meeting of the American Astronomical Society, June 1-5, 2014, Boston, Massachusetts.

Abstract Submission for oral and poster presentations opens 3 February 2014. The deadline for receipt of abstracts is 9:00 pm ET, Monday, 3 March 2014. Late abstracts will be accepted until 9:00 pm ET, Thursday, 17 April 2014. Detailed Abstract Information and Presentation Instructions can be found at:

http://aas.org/meetings/aas224/abstracts_full

Laboratory astrophysics is the Rosetta stone that enables astronomers to understand the cosmos. This will be illustrated in the meeting. Astronomy is primarily an observational science detecting photons generated by atomic, molecular, chemical, and condensed matter processes. Our understanding of the universe also relies on knowledge of the evolution of matter (nuclear and particle physics) and of the dynamical processes shaping it (plasma physics). Planetary science, involving both remote and in-situ measurements of solar system bodies, requires knowledge from physics, chemistry, and geology. Exploring the question of life elsewhere in the Universe draws on all the above as well as biology. Hence, our quest to understand the cosmos rests firmly on theoretical and experimental research in many different branches of science. Taken together, these astrophysically motivated studies are known as laboratory astrophysics. The meeting will be divided into six sessions that will focus on the interplay between astrophysics and experimental studies into the underlying atomic, molecular, dust and ice, planetary science, plasma, and nuclear processes that drive our Universe and that shape our understanding of it.

Confirmed Invited Speakers:

Bridging Laboratory & Astrophysics: Atoms
Randall Smith, Harvard Smithsonian Center for Astrophysics
Gregory Brown, Lawrence Livermore National Laboratory

Bridging Laboratory and Astrophysics: Molecules
Paule Sonnentrucker, Space Telescope Science Institute
Michael A. Duncan, University of Georgia
Bridging Laboratory and Astrophysics: Dust and Ices
Bruce Draine, Princeton University
Ral A. Baragiola, University of Virginia
Bridging Laboratory and Astrophysics: Planetary
Sara Seager, Massachusetts Institute of Technology
Larry Nittler, Carnegie Institution of Washington
Bridging Laboratory and Astrophysics: Plasmas
Chris Niemann, UCLA
Jim Bailey, Sandia National Laboratories
Bridging Laboratory and Astrophysics: Nuclear & Particles
Arthur Champagne, University of North Carolina
Johan Frenje, Massachusetts Institute of Technology

In addition to its Annual Meeting, LAD, is also holding a one-day Meeting jointly with the AAS SPD Division and the APS GPAP Topical Group in Plasma Astrophysics. The two joint sessions, Bridging Laboratory and Solar Plasma Studies I and II, will focus on the interplay between laboratory astrophysics, plasma physics and solar physics.

SOC:
Farid Salama (NASA/Ames Research Center), Chair
John Black (Chalmers University of Technology)
Nancy Chanover (New Mexico State University)
Paul Drake (University of Michigan)
Chikang Li (Massachusetts Institute of Technology)
Daniel Wolf Savin (Columbia University)
Gianfranco Vidali (Syracuse University)
Steven Federman (University of Toledo), ex-officio

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