Chemistry of asteroid Ryugu revealed by the Hayabusa2 mission

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The Hayabusa2 spacecraft made two successful landings onto asteroid Ryugu to collect asteroidal materials in 2019 and delivered the collected samples to the Earth on December 6th, 2020. The colors, shapes and macro-structures of the returned samples are consistent with those acquired by remote sensing observations indicating that the returned samples are representative of the asteroid Ryugu. The initial analyses of the samples have been recognized that Ryugu mainly consist of carbonaceous chondrites and the material is show kinship to the chemically most primitive meteorites, CI chondrites.

The characteristics are: (1) Ryugu samples show strong similarities to CI (Ivuna-like) carbonaceous chondrites in chemistry, but poor in H_2O (Fig. 1). (2) Mineralogical and physical properties of Ryugu samples occurred early to progressed aqueous alteration in its parent asteroid. (3) The macromolecules of Ryugu record various organics-water-mineral interactions during the aqueous alteration. (4) A variety of prebiotic organic molecules including amino acids were identified in Ryugu samples. (5) Ryugu grains have resided at a certain depth until sampling, and only a limited number of the Ryugu grains were exposed to solar wind irradiation. (6) Ryugu grains recovered show unique surface modifications related to space weathering.

These results show that Ryugu samples are more primitive than any CI chondrite group samples and therefore represent the most pristine Solar System material available for study. Materials observed in the CI chondrites may have been significantly changed or modified on Earth from their primary states in space. Such modification likely resulted in the alteration of the structures of organics and phyllosilicates, the adsorption of terrestrial water, and the formation of sulfates and ferrihydrites for the CI chondrites fallen on the Earth.

FINE DUST COATING ON RYUGU INDICATED BY COMPARING RYUGU SAMPLE TO IN-SITU DATA

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C-type asteroid (162173) Ryugu was thoroughly investigated by remote sensing observations with Hayabusa2 [1], and in-situ observations by MASCOT [2] and samples were successfully returned to Earth and distributed to various research institutions [3]. Here, we present a comparison of the mid-IR spectrum of sample C0137 to data obtained in the same spectral range with the MASCOT Radiometer.

Hayabusa2 revealed that Ryugu is a rubble-pile asteroid with a surface dominated by boulders and coarse gravel, despite a low overall thermal inertia derived from telescopic observations that was interpreted as fine sand-like regolith prior to arrival [1,4,5,6,7]. The full diurnal temperature curve observed by the MASCOT Radiometer revealed that the low thermal inertia is a bulk property of the boulders rather than a substantial dust layer on top of a more compact boulder [4]. Consequently, little to no dust were found on Ryugu and observations of the OSRIS-REx mission to (101955) Bennu came to the same conclusion [8,9]. The low thermal inertia of the boulders was interpreted as high-porosity material [5,6,7], while recent works indicate that cracks could also significantly reduce the thermal inertia of the materials on Ryugu or Bennu [10, 11]. It is unclear whether no or little dust is produced on these asteroids or if most of the produced dust is lost immediately.

In the presented work we find that a very thin layer of dust, maximal 55 μ m, covering a porous or cracked boulder with a thermal inertia of around 305 Jm⁻²K⁻¹s^{-1/2} can still be supported by MASCOTs observations. These results are obtained by thermophysical modelling of Ryugu's surface using a two-layer model, varying thermal inertia of the dust and the boulder, as well as the thickness of the dust layer as free parameters.

We also find a significantly reduced spectral contrast around $10\mu m$ on Ryugu compared to thin section spectra of C0137. The comparison is achieved by convolution of the mid-IR spectrum of C0137 by the MASCOT Radiometer's instrument function and subsequent analysis of the instrument's band ratios. A fine dust layer of as little as $13\mu m$ could already explain such a change in the spectrum while leaving to trace in the diurnal temperature variation and a similar explanation was found for the low contrast of the mid-IR spectra observed at Bennu [12].

The presence of dust in form of a very thin coating indicates that dust is produced on Ryugu while most of it is lost. This could make small asteroids like Ryugu and Bennu relevant sources of dust in the solar system.

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Depletion of the Interplanetary Dust Close to the Sun

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Images from the STEREO/SECCHI/HI-1 heliospheric imager (launched in 2006) and the PSP/WISPR (launched in 2018) have been used to update and extend the historical observations of the zodiacal light (ZL), (e.g., Leinert et al 1981). The recent observations from WISPR have shown a steady decrease in the brightness beginning at 19 Rsun (0.1 AU) down to about 5 Rsun where a long-postulated dust free zone begins. This result is the latest in a series of papers analyzing the SECCHI observations to prepare for the similar observations to be obtained from the Parker mission. We will also discuss the following updates to the Helios observations by Leinert:

(1) Constancy of the intensity of the symmetry axis of the ZL; (2) Extension of the exponent of the radial profile from -2.3 to -2.31 down to 0.1 AU; (3) Confirmation of a slight increase in the slope approaching the Sun; (4) Observation of the dependence of the inclination and ascending node on heliocentric distance; (5) Center of the Zodiacal Cloud offset toward the barycenter;
(6) Determination of the shape of the ZL as a function of heliocentric distance; (7) Discovery of dust in or near the orbit of Mercury; (8) Discovery of dust in or near the entire orbit of Venus.

Far-infrared Observation of the Near-Ecliptic Asteroidal Dust Band and Its Origin

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The zodiacal emission is the thermal emission from the interplanetary dust widely distributed in the solar system. It is the dominant diffuse radiation in the mid- to far-infrared (IR) wavelength region except near the Galactic plane. It was found that there are many small-scale structures in the zodiacal emission distribution, including dust band pairs at the ecliptic latitudes of $\pm 1.4^{\circ}$, $\pm 2.1^{\circ}$, and $\pm 9.3^{\circ}$, apart from a smooth background distribution. These three major dust-band pairs are now considered to be associated with the Beagle, Karin, and Veritas asteroid families, respectively. It is thought that disruption events in the main asteroid belt, which would have occurred within the last 10 Myrs, are major supply sources of dust particles. Although the $\pm 2.1^{\circ}$ and $\pm 9.3^{\circ}$ bands are well studied, there are not enough observations for the $\pm 1.4^{\circ}$ bands.

We investigate the geometry of the $\pm 1.4^{\circ}$ and $\pm 2.1^{\circ}$ dust-band structures in the far-IR all-sky maps observed with the Japanese infrared satellite AKARI. AKARI clearly detects the both dustband structures at 90 μ m. AKARI's observations detected the $\pm 1.4^{\circ}$ band structure over a wide Ecliptic longitude region, which strongly supports the Beagle family origin.

On the good way to generate a numerical analogue of fractal dust particles for optical purposes

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Standard analysis of light scattered by a cloud of dust particles comes from quantitative comparison with computer data calculated from modeled finite particles. When dust particles are expected to be fractal, the use of standard light scattering software (e.g. T-Matrix codes, DDA codes, etc.) requires the digital generation of dust particles in the form of grain aggregates for which the location of each grain is known. The corresponding Particle-Cluster or Cluster-Cluster aggregation codes are today effective up to a few millions grains per dust particle. That way, the number, N, of grains of radius a in an aggregate scales as a power law with the reduced radius of gyration of the particle, R_g/a , following: $N = k_f (R_g/a)^{d_f}$, where k_f (the prefactor) and d_f (the fractal dimension) are the parameters of the fractal morphology of the particle. Long ago, it was proven that this scaling relation was representative of a critical system, and that the fractal dimension was universal (*i.e.* d_f depends on a few parameters, such as the space dimension and the diffusion of dust particles as they form) while the prefactor was not (that is k_f depends on a multitude of details). An important consequence of the concept of universality is that it is illusory to try to reproduce the observed (real) value of the prefactor using a computer program, while the value of the fractal dimension is absolutely correct as soon as the relevant parameters are included in the model. If therefore the optical cross-sections depend on both universal and non-universal parameters (that is generally the case), light scattering programs - even if they are exact - are not able to give reliable values to compare with values observed in nature. A way around this issue is to use numerical codes generating particles of imposed fractal dimension and prefactor. Such numerical codes exist but the corresponding calculation load is heavy.

Instead of trying to reproduce the scaling law between N and R_g for a large collection of finite fractal aggregates, it is more natural to precisely model the pair-correlation function of a large fractal particle, and to use a light scattering code directly employing that correlation function as input. In this presentation we will discuss the novel method called MFT+ (for: Mean-Field Tmatrix, and + for the improved version). When we proposed the first version of that method MFT, twenty-five years ago, too schematic consideration of the pair correlation function in the domain of small distances, limited the accuracy of the method. We have recently significantly improved this part of the MFT method. Now, the values of the optical cross sections of fractal particles of any size can be calculated with good accuracy in short times. One can then obtain an estimate of the values of the optical cross sections with realistic error bars using a range of possible values of the prefactor (coming from the shape of the pair-correlation function). We will see an analysis of Titan's dusty atmosphere using the MFT+ method.

Large particles in cosmic dust

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Recent observations of different dusty objects (disks, comets, active asteroids) show an abundance of dust particles in the size range of hundreds of microns and even millimeters. Evidence of this is in situ data for comets and asteroids; also, they show unusual photometric and polarimetric properties, specifically, their phase curves are very different from those considered typical for cosmic dust. Laboratory measurements of large particles (Munoz et al., Astroph. J. Suppl. Ser., 247, 19, 2020) showed that the unusual phase curves can be characteristics of mm-size particles. However, the most popular computational techniques that model light scattering by dust particles (e.g., T-matrix, DDA) are not capable to simulate the photopolarimetric properties of particles of size larger than 10-20 microns as the computations for such particles are too demanding to the computer resources and cannot be handled even with modern supercomputer clusters.

In this presentation, we consider new techniques recently developed to model light scattering by large particles to overcome the computational problems. Specifically, we describe a multi-sphere superposition method for large-scale systems based on an accelerated T-matrix algorithm (Mackowski and Kolokolova, JQSRT, 287, 108221, 2022) and its results that allow seeing some regularities in light scattering by large aggregates depending on their material, number, and size of spheres. We will also introduce the Fast superposition T-matrix method (FaSTMM) which uses the fast multipole method (FMM) to speed up the superposition T-matrix solution (Markkanen and Yuffa, JQSRT, 189, 181, 2017). The FMM forms monomer groups hierarchically and computes electromagnetic interactions between the separate groups at each level of the hierarchy. FaSTMM code is available at https://wiki.helsinki.fi/display/PSR/. FaSTMM was successfully used to model large dust particles in the coma of comet 67P/Churyumov-Gerasimenko and could successfully reproduce its unusual photometric phase curve (Markkanen and Agarwal, Astron. Astrophys. 631, A164, 2019). It also successfully reproduces the photometric and polarimetric phase curves observed for the disk HR 4796a (Arriaga et al. Astron. J., 160.2, 2020).

We will present photopolarimetric observations of comet C/2014 B1 (Schwartz) at 9.6 au and show that the FaSTMM simulations of its polarization, color, and their change within the coma require particles of size up to several millimeters.

Polycyclic Aromatic Hydrocarbon Molecules in Comets

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Polycyclic aromatic hydrocarbon (PAH) molecules, ubiquitously seen in the interstellar medium (ISM) of our own and external galaxies, might have been incorporated into comets if they are formed from relatively unprocessed interstellar matter. The detection of PAHs in comets would be an important link between the ISM and comets and the solar system formation. While there is yet no definite detection in comets of the infrared (IR) emission features at 3.3, 6.2, 7.7, 8.6 and 11.3 um which are commonly attributed to PAHs, small PAHs (naphthalene $C_{10}H_8$, phenanthrene $C_{14}H_{10}$, pyrene C₁₆H₁₀, perylene C₂₀H₁₂) have been found in the *Stardust* samples collected from comet 81P/Wild 2, in the Rosetta samples collected from comet 67P/Churyumov-Gerasimenko, and in interplanetary dust particles possibly of cometary origin. In principle, IR spectroscopy could also provide identification of these small molecules, provided that they are sufficiently abundant and the telescope instrument is sufficiently sensitive. With the advent of the James Webb Space Telescope (JWST), this may become possible due to its unprecedented sensitivity. With an aim to offer spectroscopic guidance for JWST to search for these PAH molecules in comets, we model the vibrational excitation and calculate the IR emission spectra of these small PAH molecules in cometary comae, illuminated by the Sun at a range of heliocentric distances ($r_h = 0.5, 0.75, 1, 1.5, 2$, 3, 5 AU). By comparing the observed IR emission spectra of comets with the model spectra, one will be able to derive (in case of detection) or place an upper limit on (in case of nondetection) PAH production rates in comets.

The stucture of dusty debris disks

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Minor bodies similar to asteroids and comets are ubiquitous components of planetary systems, typically found in belts analogous to the Asteroid and Kuiper belt in the Solar System. Although we cannot detect these bodies individually, mutual collisions between km-sized planetesimals produce high dust levels that are readily detectable in cold belts around 30% of nearby stars that we call debris discs. These belts provide unique and complementary constraints on the formation, architecture, and dynamics of planetary systems. In this talk I will review how over the last 5 years using ALMA observations we have been able to constrain the radial and vertical structure of exoKuiper belts, providing unique information about how planetesimals form and the dynamics in the outer regions of planetary systems. These efforts have opened a window into the outer regions of planetary systems that is complementary to exoplanet surveys and planet formation studies.

What is hot dust doing so close to main-sequence stars?

Excess near-infrared emission is detected around one fifth of main-sequence stars, but its nature is a mystery. These excesses are interpreted as populations of small, hot dust very close to their stars, but such grains should rapidly sublimate or blow out of the system. Many models have been put forward to explain this phenomenon, but to date, none has successfully explained the nature of hot dust, nor its ubiquity around such a diverse range of star types and ages. The fundamental problem is that it is unclear how to deliver and sustain these dust populations, which comprise grains small enough and hot enough for their near-infrared emission to significantly exceed their mid-infrared emission. I summarise the current status of the field, including what we do and do not know from observations and recent theoretical work. I give an overview of the diverse range of models seeking to explain hot dust, and particularly focus on how upcoming observations with VLTI/MATISSE should significantly improve our understanding. I also discuss areas where further progress must be made if we are to explain the phenomenon. My aim is to motivate input from the broader dust community, to identify any physics that we may have overlooked, and identify promising new directions in our attempts to explain hot dust.

Importance of Collisional Sticking of Fine Particles in Debris Disks

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High-velocity (several hundreds m/s) collisions in planetary siystems are believed to lead to collisional fragmentation. Once collisional fragmentation of kilometer-sized or larger planetesimals occurs, the collisional cascade grinds down to micron-sized or smaller dust grains, which are shortly removed by the radiation pressure or other effects. Therefore, the size distribution of dust grains are naturally determined by the quasi steady state evolution in collision cascades, which show simple power law distributions. Debris disks are formed from collisional cascades. Their spectral energy distributions (SEDs) are mostly determined by the size distribution because debris disks are optically thin. However, some SEDs of debris disks require the size distributions much steeper than those given by collisional cascades. To reconcile it, the artificial reduction factor for the sub-millimeter fluxes was used for debris-disk SED fittings (e.g., Wyatt 2008).

Recent laboratory experiences show such collisions of micron-sized or smaller fine particles result in sticking. Taking into account collisional sticking, we carried out simulations of collisional evolution in debris disks. We find collisional evolution with sticking results in a steeper size distribution.

We perform collisional evolution simulations considering the debris disk around HD114082. The disk is shaped as a ring and its radius and width are obtained through high resolution observations (Wahhaji et al 2016). Therefore, it is a good target to test the collisional model with sticking. We calculate the SEDs according to the resultant size distributions. A simple power law distribution with index -3.5 explains the fluxes in ~ 10–100 μ m, while it overestimates the flux at longer wavelengths. The result of collisional evolution without sticking is better than the overestimate in the simple power law case, but the flux at $\gg 100 \,\mu$ m is overestimated. The result with sticking is most likely to explain the SED.

Therefore, collisional cascades with sticking result in steeper size distributions for millimetersized or smaller dust grains. This modification may naturally explain the reduction of (sub)millimeter fluxes in debris disks.

An Analytic Expression for the Impact Strength of Porous and Nonporous Solid Particles in the Size Range from Nanometers to Kilometers

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The presence of our planet Earth and life on the planet provides strong evidence that a mutual collision of two bodies (e.g., dust, pebbles, and planetesimals) in protoplanetary disks does not necessarily result in catastrophic disruption but it could assist in coalescence of the bodies into a planet. The outcome of mutual collisions can be predicted, provided that in advance of the collisions we acquire considerable knowledge of impact strength, which is defined as the total kinetic energies of an impactor and a target per unit target mass when the mass ratio of the largest fragment to the pre-impact target is exactly one half. Since the impact strength of colliding bodies is the main determinant of planet formation, a thorough study on the impact strength of porous and nonporous particles is crucial to better understanding the formation of planetary systems. It is, however, worthwhile noting that such a study has been so far restricted, to a large extent, to laboratory experiments with various physical and chemical properties of solid bodies. Therefore, we devote ourself to a theoretical investigation of impact strength based on Johnson-Kendall-Roberts theory of contact mechanics, Griffith theory of fracture mechanics, and Weibull theory of flaw statistics. Here, we propose an analytic expression for the impact strength of porous and nonporous solid particles that is capable of reproducing experimental results in the literature, regardless of the particles are aggregates or monoliths. It gives straightforwardly theoretical estimates of impact strength, provided that the volumes or radii of colliding particles, the volume fractions of solids in the particles, the surface energies, Young's moduli, Poisson's ratios, and densities of the solids, the radii of constituent monomers, and the Weibull moduli or the maximum flaw lengths of the particles are known. We will not only demonstrate how well the analytic expression explains experimental results with icy and siliceous materials but also discuss how the impact strength should vary with the size and porosity of particles, and, if the same material is considered, with the volume ratio of the particles.

Inferring the Solid Composition of Disrupting Minor Planets in White Dwarf Dusty Disks from Infrared Spectra

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Revealing the source materials of planets is important for understanding the interior of solid exoplanets that are ubiquitously found beyond our solar system. Between a quarter and half of white dwarfs have metals in their atmospheres (e.g. Zuckerman et al., 2010), and some of them exhibit an infrared excess from their circumstellar dusty discs (Rocchetto et al., 2015). These are thought to originate from minor planets that survive their host stars' post-main-sequence evolution and are subsequently disrupted around white dwarfs. Therefore, observations of metals in and around white dwarfs could provide a unique opportunity to probe the solid composition of minor planets.

If we can determine the mineral composition of dust particles in the disks around white dwarfs through their thermal emission spectra, we could infer the composition of disrupted minor planets. In fact, noticeable silicate features have already been detected in several disks, and Reach et al. (2009) constrained the candidate dust composition for the disk around G29-38 based on its observed infrared spectra. However, they did not investigate which particle sizes and disk geometries determine the observed spectra's profile. While Ballering et al. (2022) studied the dependence of spectra on such disk parameters, they fixed the dust composition at a hypothetical mineral, astronomical silicate.

In this study, we consistently investigate the impacts of dust mineral composition and disk parameters on spectra. We use a simple analytical two-layer model of passive disks (Chiang et al. 2001) to calculate the thermal emission spectra of the disk around G29-38. When comparing the calculated spectra to the observed ones, we focus on (1) the silicate feature at 10 μ m and (2) the gentle excess peak at 5 μ m. First, as Ballering et al. (2022), we calculate the spectra assuming dust composed of the hypothetical material, astronomical silicate. We find that the emission from particles on the disk surface at ~1000K governs the spectra profile. Furthermore, particles smaller than 5 μ m produce (1) while larger particles than ~5 μ m contribute to (2). We then recalculate the emission spectra using optical data of existing amorphous silicates, iron metal, and amorphous carbon (Dominik et al. 2021). We find that dust consisting solely of silicate cannot reproduce the shape of (2) even if changing disk parameters. On the other hand, the mixture of pyroxene silicate and amorphous carbon can well reproduce both (1) and (2). The best-fit composition allows a wide range of Mg/Fe ratios for pyroxenes but limits carbon fraction to 3-4wt%, implying that the disk originated from planets with C-type asteroid-like elemental composition. In this presentation, I will also discuss the results of the analysis of other white dwarf disks whose infrared spectra have been observed.

Infrared Emission Spectra of R Coronae Borealis Stars

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The R Coronae Borealis (RCB) stars are a small group of carbon-rich, hydrogendeficient super-giants. RCB stars often show unusual variabilities in the optical, which are commonly thought to be caused by the formation of carbon dust at irregular intervals. *Spitzer*/IRS and AKARI spectroscopic observations of RCB stars have revealed a complex dust chemistry. While several RCB stars exhibit well defined PAH emission bands at 3.3, 6.2, 7.7, 8.6, and 11.3 μ m, the vast majority shows broad, unidentified emission complexes at ~6--10 μ m and ~11.5--15 μ m. We model the infrared emission of RCB stars and try to understand the nature of the dust condensed in RCB stars.

Red Stars over PAHs

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Polycyclic aromatic hydrocarbon (PAH) molecules are widely considered to be responsible for the 3.3, 6.2, 7.7, 8.6, 11.3, and 12.7 µm emission bands, collectively known as the "unidentified" infrared emission (UIE) bands. One argument often invoked to argue against PAHs as the carriers of the UIE bands is that, the excitation of PAHs is thought to require ultraviolet (UV) photons and therefore, the PAH model is thought to fail in explaining the presence of UIE bands in UV-poor regions (e.g., reflection nebulae and proto-planetary nebulae where the central stars are cool). However, it has also been argued both theoretically and experimentally that the excitation of PAHs does not require UV photons. To explore whether PAHs can be excited sufficiently in UV-poor regions to emit at the UIE bands, we investigate the vibrational excitation of PAHs in circumstellar envelopes around cool carbon stars. These stars have an effective temperature of $T_{eff} < 6000$ K and the UIE emission has been detected in their circumstellar envelopes. To this end, six such stars were selected, i.e., IRAS Z02229+6208, IRAS 20000+3239, IRAS 22272+5435, IRAS 22574+6609, IRAS 23304+6147, W Orionis, and IRAS 13416-624. We model the PAH excitation in these UV-poor systems and calculate the PAH model emission spectra. It is found that, in general, PAHs can be excited sufficiently in these systems to account for the observed UIE emission. We determine the PAH size, charging fraction, and mass and discuss the PAH chemical structure for each of these six UV-poor systems.

The Physics of the Dusty Spirals of Wolf-Rayet Binaries Revealed by Observations of WR140

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Classical Wolf-Rayet stars are the final phase of evolution of the most massive stars before they become supernovae. Their extremely high luminosities drive fast, dense stellar winds that are sometimes rich in carbon. Despite this harsh circumstellar environment, Wolf-Rayet stars can sometimes precipitate the right conditions to form large amounts of dust. One way in which this could occur is via stellar wind collisions if the Wolf-Rayet star is found in a binary. Imaging campaigns have revealed that under this mechanism, dust shells form in spectacular shapes sculpted by the orbit of the binary. We recently analysed a series of images of the dust produced by the Wolf-Rayet binary WR140 over 17 years. These images enabled us to model the geometry of the dust shell and track its motion. Surprisingly, our analysis revealed the dust to be accelerating, which likely constitutes a first direct witness of stellar radiation pressure accelerating matter in the circumstellar environment. I also discuss recent JWST ERS observations of the system, which detected a stunning series of 20 concentric dust shells spanning two light years, visualising the role of Wolf-Rayet binaries in enriching the dust content deep into the interstellar medium. The structure of these dust shells which have reached terminal velocity shows high repeatability and is well-explained by the geometry of dust produced under a colliding-wind mechanism, tracing the surface of a conical spiral. In addition to recent findings focussed on WR140, I also provide a brief overview of colliding-wind Wolf-Rayet binaries and discuss some outstanding questions that future observations and theory may wish to investigate.



Left: Keck observations showing the expansion of the inner dust shell of WR140 (Han et al. 2022). Right: JWST observations of a series of concentric dust shells of WR140 (Lau et al. 2022).

Title: Dust Aggregation in Circumstellar Shells around Oxygen-rich Asymptotic Giant Branch Stars Authors: J.A. Paquette¹ (presenter), F. T. Ferguson², and J.A. Nuth³

Abstract: The aggregation of dust in circumstellar shells around oxygen-rich Asymptotic Giant Branch stars has often been considered to be of negligible importance, because the aggregation process is strongly dependent on particle density. The number density of dust grains was thought to be too low for aggregation to have any significant effect. Recent work (Kimura et al., 2022) shows that the assumed perfectly efficient grain growth is unrealistic, with most monomers that strike a grain failing to adhere. This tends to lead to a larger number of smaller grains. In addition, the grains that form under these conditions should be very open, with a fractal-like structure, so fractal aggregation rather than Euclidean coagulation should be considered. A third item that must be taken into account is the near ubiquity of planetary systems (Batalha, 2014; Ford, 2014; Marcy et al., 2014). The presence of a planetary system will likely increase the SiO concentration in a star's outer envelope as Poytning-Robertson drag causes dust to drop into the star and evaporate. In this work we begin with nucleation of SiO dust as described by classical nucleation theory (Becker & Döring, 1935), using a simple model (Paquette et al., 2011) and compare the resulting density distributions assuming no coagulation, or Euclidean coagulation with both efficient and inefficient grain growth and inefficient grain growth with fractal aggregation. Cases with increased SiO mass fraction (to model the effects of a planetary system) are also considered. Far from being negligible, we show that under conditions of inefficient grain growth and fractal aggregation the dust number density distribution is dramatically changed, in a way that potentially promotes acceleration of dust grains by radiation pressure.

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Modeling dust formation in supernovae in the JWST era

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The formation of molecules, molecular clusters, and their transition to solid grains of dust, control the chemical budget of supernovae (SNe) from their nebular phase to the remnants. By quantifying the mass and composition of dust in SN ejecta, we develop tools that enable us to study the hydrodynamics of the SNe, in terms of the nature of the explosion, geometry of the ejecta, the mass of the ejecta, pre-explosion activities of the massive star, degree of mixing and clumpiness of the layers induced by the explosion. Based on the type of progenitor, theories predict the dominance of C-rich (expected in smaller progenitor stars) or O-rich dust components (expected in larger progenitors). Moreover, the timescales of dust formation for individual species differs based on the densities of the clumps and the cooling rates defined by elements present in those clumps. In recent years, we have realized that the interaction of the SN shock with circumstellar environments influence the physical and chemical evolution of the SN profusely. In many interaction-dominated SNe, dust is assumed to form in the post-shock gas (behind the SN blast wave), with a larger survival rate when merging with the ISM.

The molecules are crucial in determining the pathways to form various dust grains, in addition to being responsible for the rapid cooling of the gas. Possibility of detection of molecules in extragalactic SNe, decades after the explosion, provides the critical evidence for determining the pathways of dust formation. In addition, tracing the rate of dust production until late times helps us understand the mechanism of dust growth, which is connected to the compactness of the core and the mantle of these dust grains. The destruction of these grains by the reverse shock is affected by this outcome.

At any given time, the range of dust temperatures in SNe can vary over a wide range, thereby radiating at all wavelengths from near-IR to submm wavelengths. Several evidence points towards the likely presence of large masses of cold dust, however prior to the JWST era we had no tools to test that. Thanks to the ongoing detections of dust reservoirs in several extragalactic supernovae, using the mid-IR data from the JWST, we now have a much improved understanding of the role of SNe as dust producers in galaxies.

In my talk, I will present the current state-of-the-art in the field of supernova dust, explaining the physics and chemistry of dust formation in such environments and their observational consequences.

Study of dust in novae environment

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Novae are the only objects in which it has been possible to observe directly all aspects of circumstellar grain formation on a frequent basis. Compared to interstellar dust, novae dust forms within a short time frame of 30 to 100 days after an outburst, allowing them to serve as test beds for understanding the formation and evolution of astrophysical dust. However, dust formation in the hostile environment of novae ejecta has been an open question for many decades. Several attempts have been made to understand the physical and chemical conditions required to dust formation in novae ejecta and its relation with the observable parameters. In this work, we have studied the dust forming nova V1280 Scorpii (2007) with the aim to study the evolution in the physical and chemical parameters. We model the predust and postdust phase optical and near-infrared spectra using the photoionization code CLOUDY, v.17.02, considering a two-component (low-density and high-density regions) model. It is found that a very high hydrogen density ($\sim 10^{13} - 10^{14} \text{ cm}^{-3}$) is required for the proper generation of spectra. Dust condensation conditions are achieved at high ejecta density (~ 3.16×10^8 cm⁻³) and low temperature (~ 2000) K in the outer region of the ejecta at a distance, $R \sim 4.07 \times 10^{15}$ cm away from the central ionising source. A mixture of small $(0.005-0.25 \ \mu m)$ amorphous carbon dust grains and large $(0.03-3.0 \mu m)$ astrophysical silicate dust grains are present in the ejecta. Our model also yields very high elemental abundance values as C/H = 13.5-20, N/H = 250, O/H = 27-35, by number, relative to solar values, during the preduct phase, which decreases in the postdust phase.

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Physicochemical Processes on Cosmic Ice Dust

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Physicochemical processes on cosmic ice dust are indispensable for chemical evolution at each stage of star formation. The chemical evolution begins in molecular clouds where temperature is as low as 10 K. In molecular clouds, the hydrogenation of primordial atomic and molecular species plays an important role because hydrogen atoms can migrate and encounter reaction partners on the grain surface even at ~10 K. The formation of abundant interstellar species like H₂O, NH₃, H₂CO, and CH₃OH by reactions often through quantum tunneling on the cryogenic ice surface was experimentally confirmed [1, 2]. Furthermore, hydrogen-deuterium substitution reactions on ice dust were found to promote deuterium enrichments of interstellar molecules. Apart from these chemical processes, nuclear spin, in other words ortho-to-para state, conversion of H₂ is crucial for not only chemical evolution but also gas dynamics toward star formation because H₂ in the ortho-ground state (J=1) is more energetic and thus reactive than that in the para-ground state (J=0) by approximately 14.6 meV corresponding to 170 K. The radiative transformation of molecular nuclear spins is forbidden in the gas phase but not on the dust surfaces. We experimentally observed the nuclear spin conversion of H₂ on various types of dust analogues [3].

Recently, significant progress in astronomical observations has enabled us to discover many kinds of complex organic molecules (COMs), in particular, towards star-forming regions. During temperature elevation in star-forming regions, heavier species can diffuse on the ice dust and subsequently many COMs would be produced through reactions among heavier species, especially radicals. It is thus important to investigate experimentally the behavior of radicals on the ice surface for understanding formation pathways of COMs. However, conventional methods for detecting OH radicals on ice, such as Raman, infrared, and electron spin resonance spectroscopies, are not applicable because of their low detection sensitivities and non-surface selectivity. We recently developed a new method, a combination of photostimulated desorption (PSD) and resonance-enhanced multiphoton ionization (REMPI), for directly detecting radicals on ice at low temperatures [4]. Using the PSD-REMPI method, the activation energies for diffusion of OH [5] and C radicals on ice were determined.

In about two decades, our group at ILTS has revealed various physicochemical processes related to above mentioned phenomena. In my talk, some of our experiments including their astronomical backgrounds will be presented.

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ALMA observations of peculiar embedded icy objects found by the infrared satellite AKARI

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Two peculiar embedded icy objects were found by the infrared satellite AKARI in the Galactic plane direction (Onaka et al. 2021, ApJ, 916, 75). Both objects show deep ice absorption features that are often seen in embedded young stellar objects (YSOs) or background stars sitting behind dense clouds, however, they are located neither in known star-forming regions nor in known dense clouds. Their infrared SEDs show a peak around 5 micron, which are incompatible with existing SED models of embedded YSOs. If they are truly YSOs, similar objects should have eluded past photometric surveys, which would require a revision of our view of the distribution of YSOs in our Galaxy. If they are background stars, there must be dense and very compact starless clouds in the line-of-sight, which have eluded past dense cloud surveys, or ice species may grow in unknown processes in tenuous clouds. Either case will make a significant impact on our understanding of the ice chemistry and/or star-formation process in our Galaxy.

To reveal their nature, we recently carried out submillimeter observations with ALMA (12m+ACA). Very compact emission of CO(3-2) and SiO(8-7) are detected at the positions of two icy objects. The observed large integrated intensity ratios of SiO(8-7)/CO(3-2) (\sim 0.3-0.4), as well as their broad line widths (8-15 km/s), imply the contribution from shocked gas. Although a large dust extinction (Av \sim 80-120 mag) is expected from their deep dust/ice absorption bands, no dust continuum emission is detected, which would suggest a large beam dilution effect due to the compact size of the sources. Their systemic velocities are clearly separated from the surrounding CO clouds, suggesting that they are isolated.

These characteristics of the SEDs, the presence of deep dust/ice absorption features, and compact SiO-dominated broad molecular line emission, cannot easily be accounted for by standard YSO models. They may be explained as isolated, shock-dominated, edge-on disk sources without thick envelope, but detailed modeling is necessary. I will discuss possible nature of those icy objects.

Multi-Band Far-Infrared Polarization as a Means of Recovering 3D Information on Interstellar Magnetic Fields and Grain Alignment

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The polarization of far-infrared (FIR) dust emission is one of the most important tracers of interstellar magnetic fields, as well as dust properties themselves. This because interstellar dust grains are generally non-spherical and their major axes tend to orient perpendicularly to magnetic field lines. Since emission is preferentially polarized along a grains' longer axis, the polarization angle of dust emission contains information on the magnetic field's projected direction on the plane of the sky. Furthermore, the polarization fraction is often used to estimate magnetic field disorder and grain alignment efficiency. Polarimetry is therefore central to many astrophysical fields, including star formation and galaxy evolution on cosmic times.

Unfortunately, there are two major limitations to the efficiency of polarization as a tracer. The first is that it can only provide information on the projected magnetic field, with a loss of information on the 3D structure of the magnetic field. Secondly, polarization fraction is degenerate: in typical observations, one cannot separate the effects of magnetic field structure, grain alignment and dust optical properties, so that the polarization fraction provides limited information by itself.

Both of these problems can be alleviated by using multi-band FIR polarimetry, as opposed to single-band. In environment with strong temperature gradients on the line of sight – such as molecular clouds – different bands are sensitive to dust at different temperature, and therefore in different cloud regions. In environment with relatively uniform temperatures, such as the diffuse interstellar medium, it can be shown that the effects of magnetic fields on polarization are at first approximation independent of wavelength: the shape of the polarization spectrum is then a good constraint on the dust properties and alignment.

I will present our team's results for a pilot study of multi-wavelength polarization in the starforming region NGC 2071. The analysis combined 850 μ m data from POL-2 at JCMT (observed as part of the BISTRO survey) with 154 and 214 μ m data from HAWC+ on SOFIA. We detect a wavelength dependence of the polarization angles on a significant fraction of the target; this is most likely caused by a rotation of the magnetic field lines within the cloud. On those regions where the observed polarization angle is constant, the polarized spectrum shape suggests heterogenous grain alignment within the cloud. Overall, the analysis shows the potential of multi-band polarimetry for tracing the 3D structure of magnetic fields, as well as grain alignment.

I will also discuss the planned follow-ups to this analysis, including the selection of new polarimeters and databases following the decommissioning of SOFIA, the challenge of combining data from different telescopes, and the techniques we developed to improve our inter-telescope comparison.

Investigating Multi-wavelength Signatures of the Quiescent Molecular Cloud, DC 314.8–5.1

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DC 314.8-5.1 is a quiescent molecular cloud prior to the onset of star-formation. It is unique due to a coincidental association with a B-type field star, which illuminates a reflection nebula within the cloud, resulting in infrared emission from the dust grains, specifically Polycyclic Aromatic Hydrocarbons (PAHs). The study of the individual PAH features showed that the system displays differing characteristics from similar systems with reflection nebula incident from star formation. Additionally, the emission indicated a higher than expected ionization level of the system, potentially due to cosmic-ray interactions. In addition to the uniqueness of the system with respect to its companion star and its evolutionary stage, DC 314.8-5.1 is particularly well suited for multi-wavelength investigation because of (i) its proximity (432 pc), and (ii) its location below the Galactic Plane.

In this work, we present an analysis of the multi-wavelength observations of the dark globule, DC 314.8–5.1, using the optical survey Gaia, the near-infrared survey 2MASS, the mid-infrared survey WISE, dedicated imaging with the Spitzer Space Telescope, and X-ray data obtained with the Swift-XRT telescope. For this purpose, we studied the infrared colors, optical parallax, and x-ray emission of all point sources coincident within the boundaries of the cloud. Ultimately we found no candidate sources down to a a mass of $0.01 M_{\odot}$ for Class I–III YSOs and to a Swift-XRT (0.5–10 keV) luminosity level $\leq 10^{31} \mathrm{erg s}^{-1}$.

Our detailed analysis of the gathered multi-wavelength data confirms a very young, "pre-stellar core", evolutionary stage of the cloud, supporting the claim that the high ionization level may be the result of cosmic-ray interactions. All in all, our analysis indicates that DC 314.8-5.1 constitutes a compact reservoir of cold dust and gas, providing a truly unique insight into a primordial form of the interstellar medium.

3D Structure and Extinction Law of Nearby Molecular Clouds

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Molecular clouds (MCs), as the star birthplaces, are generally dense that causes high extinction. A precise estimation of the extinction is crucial to revealing the true brightness and color of the stars embedded and behind the cloud. In addition, molecular clouds are place for dust growth. The determination of the extinction law of MCs would help understand the dust evolution in various star-forming environments. The nearby MCs to be studied in this work, specifically the Taurus MC (hereafter TMC), Orion MC (OMC), Perseus MC (PMC) and California MC (CMC), represent different including massive and low-mass star-forming environments. With precise measurements and large quantity of tracers, the extinction of MCs can be calculated with high precision for each MCs, and therefore serve as the references of extinction for star forming regions.

The data are based on the LAMOST and APOGEE spectroscopy with photometry data from FUV band of GALEX to W3 band from WISE. Extinctions are calculated from color excess derived from the Blue Edge methods. In combination with the distance from the Gaia, a 3D extinction map and the structure of these MCs can be retrieved and the clouds that overlap in the sky area can be separated. Also, the differences of extinction law in each MCs are studied from UV band to IR band, demonstrating the different interstellar environment in different MCs.

Mineralogical properties of dust in heavily obscured AGNs and their implications for the evolution of circumnuclear material

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In general, many of active galactic nuclei (AGNs) in their early evolutionary phases are deeply embedded in and heavily obscured by dense clouds in the circumnuclear regions. In such early phases, the activity of AGNs is usually quite high, and thus expected to significantly influence the physical and chemical properties of the material surrounding AGNs through mechanical shocks by energetic jets and irradiation by high-energy photons. The properties of the material thus influenced, in turn, can be an important probe to investigate obscured AGN activity and even trace back the history of the activity.

In this study, we aim to obtain mineralogical properties of silicate dust in nearby heavily obscured AGNs systematically, using the Spitzer/IRS 5 - 30 μ m low-resolution spectral data. We selected the sample from the archival data by the following three criteria: (1) the apparent optical depth of the 10 μ m silicate feature larger than 1.5, (2) the equivalent width of the 6.2 μ m PAH feature smaller than 270 nm and (3) the redshift lower than 0.35. The sample thus selected comprises the mid-IR spectra of 98 heavily obscured AGNs, which are fitted by semi-physical models using a one-dimensional radiative transfer calculation with four dust species of different sizes and porosities. The opacity of the dust is calculated in detail, based on the laboratory optical data of amorphous olivine, amorphous pyroxene, crystalline olivine and amorphous carbon.

As a result, our models reproduce all the spectra notably well over the broad wavelength range of 5 - 30 μ m. We find that 95 out of the 98 AGNs prefer a porous silicate dust model with absence of micron-sized large grains. The mineralogical parameters of the silicate dust derived by the fitting vary significantly from AGN to AGN; the mass ratio of amorphous pyroxene to total amorphous silicate is distributed between 0 - 40%, while that of crystalline to total silicate is between 0 - 14%. For the pyroxene mass fraction, the median and the 84 percentile of the distribution are 5.1% and 11.6%, respectively, which are significantly lower than 17%, a value typical of the diffuse ISM in our Galaxy. For the crystalline mass fraction, those are 5.8% and 8.2%, which are significantly higher than 1.4%, a value along the line of sight toward Sgr A* in our Galaxy. Overall, high porosity, small sizes, pyroxene-poor composition and high crystallinity are obtained for mineralogical properties of the silicate dust in heavily obscured AGNs. Those trends suggest that much of the dust is newly formed one originating from recent circumnuclear starburst activity, some of which has undergone crystallization processing through AGN activity.

In this presentation, we discuss the implications of the mineralogical properties of the silicate dust derived from the low-redshift bright sample of the 98 heavily obscured AGNs for the evolution of the circumnuclear material and also for that of the heavily obscured AGNs themselves. For further studies, we expect JWST for fainter AGNs and future far-IR missions like PRIMA (PRobe far-Infrared Mission for Astrophysics) for higher-redshift AGNs.

Observational evidence of morphological quenching in dusty elliptical galaxies

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The mechanism by which galaxies stop forming stars and get rid of their interstellar medium (ISM) remains elusive. I will present analysis and results obtained on a sample of more than two thousand elliptical galaxies in which dust emission has been detected. This is the largest sample of such galaxies ever analysed. One of the main result is the timescale for removal of dust in these galaxies and its dependency on physical or environmental properties. This timescale does not depend on environment, stellar mass or redshift. Another interesting result is a departure of dusty elliptical galaxies from the star formation rate vs. dust mass relation. This is caused by the star-formation rates declining faster than the dust masses and indicates that there exists an internal mechanism, which affects star formation, but leaves the ISM intact. Morphological quenching together with ionisation or outflows caused by older stellar populations (supernova type Ia or planetary nebulae) are consistent with these observations.

Dust millimetre emission in Nearby Galaxies with NIKA2/IRAM-30m: major challenges and latest results of the IMEGIN Large Program.

L. Pantoni^{1,2}, F. Galliano¹, S. Madden¹, and NIKA2 collaboration.

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The millimetre part of the spectrum is one of the least explored parts of a galaxy's spectral energy distribution (SED), yet it contains emission from three fundamentally important physical processes. These processes are thermal emission from dust, free-free emission from ionized gas and synchrotron emission from relativistic charged particles moving in the galactic magnetic field.

The NIKA2 camera (IRAM-30m telescope), observing at 1 mm and 2 mm, provides additional data points for input into the comprehensive SED models and allows us to:

- 1. disentangle spatially resolved galaxy SEDs from dust contribution, free-free and synchrotron emission;
- 2. constrain the evolution of the dust-to-gas mass ratio within galaxies, which provides a direct link to the chemical evolution of galaxies and the reservoirs for dust production;
- 3. study the microscopic properties of dust, i.e. constraints on millimetric opacity;
- 4. study the sub-millimeter excess in galaxies, whose origin is still unknown.

These are some of the main objectives of the IMEGIN Large Program (Interpreting the Millimetre Emission of Galaxies with IRAM-NIKA2; PI S. Madden), targeting 22 nearby galaxies in the millimetre continuum regime with the NIKA2 camera.

In my talk, I will present the main and latest results of the IMEGIN collaboration, which gathers researchers from 7 institutes in France (CEA, IAP, IRAM, LAM, IRAP, IAS, IPAG), and other 7 abroad (Athens observatory, University of Ghent, IPM/Iran, STScI, Calar Alto Observatory, Nat. University of Ireland, University Cardiff). The NIKA2 millimetre data, combined with a suite of observations at other wavelengths (from multi-wavelength catalogs such as Dustpedia [1]; CO and HI surveys, e.g. [2], [3]), allow us to model the IR-to-radio SED and to put constraints on interstellar medium and dust grains properties of galaxies.

Our SED analysis (performed globally and locally) makes use of the state-of-the-art hierarchical bayesian fitting code HerBIE [4], [5] with the prescriptions of the dust evolution model THEMIS, that is anchored to the laboratory-measured properties of ISD analogues [6].

During my presentation, I will focus on the major challenges linked with data processing and uncertainty propagation; large scale emission filtering in NIKA2 maps (due to atmosphere subtraction during data reduction process); latest significant results on NGC891 (Katsioli et al. in prep.) and NGC4254 (Pantoni et al. in prep.); ongoing projects (Ejilali et al. in prep. and Nersesian et al. in prep.) and future perspectives/applications.

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Kpc-scale properties of dust temperature in terms of dust mass and star formation activity

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We investigate the impact of local physical environment on dust temperature. In Hirashita and Chiang (2022), we built two analytical models for dust temperature and showed that the two most important quantities that set dust temperature are the star formation rate surface density ($\Sigma_{\rm SFR}$, tracing dust heating) and the dust-to-gas ratio (D/G, tracing dust shielding). In this work, we compile multi-wavelength observations in 46 nearby galaxies, measure their dust temperature and local physical quantities at 2 kpc resolution, and compare our measurements to the model predictions (Chiang and Hirashita et al. 2023).

We confirm that to first order, dust temperature scales with Σ_{SFR} with a correlation coefficient of 0.89, which is consistent with the model prediction. Meanwhile, there is no single quantity that traces the variation of dust temperature at fixed Σ_{SFR} throughout the entire sample space. Unlike the model prediction, we find that D/G only works as a secondary tracer of dust temperature at $\Sigma_{\text{SFR}} \gtrsim 2 \times 10^{-3} \text{ M} \odot \text{ yr}^{-1} \text{ kpc}^{-2}$. We also find that in the low- Σ SFR regime, the observed dust temperature is higher than the model predictions.

The discrepancy between the model and observations can be resolved if we modify the model to include the contribution of the old stellar population to dust heating. In our sample space, dust heating contributed by old stars becomes more important as we move to the low- $\Sigma_{\rm SFR}$ regime. This modification would improve the model prediction of dust temperature, especially in quiescent galaxies and non-starforming regions.

Finally, when comparing all the quantities implemented in the model with observations, we notice that at fixed gas surface density (Σ_{gas}), the observed Σ_{SFR} tends to be higher than the model at larger D/G. This is mainly because we assumed the standard Kennicutt-Schmidt law (K-S law) in setting up the Σ_{SFR} - Σ_{gas} relation in the model, which does not match the observation. We therefore propose an empirical correction to the K-S law with D/G and use it to improve the model prediction. The fundamental dependence of this D/G correction is likely based on the correlation between D/G, metallicity, and the HI/H₂ ratio.

Dust depletion of metals from local to distant galaxies: the origin of dust

Christina Konstantopoulou

April 21, 2023

The cycle of metals between dust and gas plays a fundamental role in the chemical enrichment of the ISM. Metals are missing from the observable ISM gas phase because they are instead incorporated into dust grains, an effect we call dust depletion. This effect alters the observed chemical abundances, which can be inferred through absorption-line spectroscopy. Characterizing the dust depletion of metals both in the local and distant Universe is important to investigate the evolution and origin of metals and dust through cosmic time. The fraction of metals in dust can be described by the dust-to-metal ratio (DTM) and the dust content by the dust-to-gas ratio (DTG). These properties can give us clues about the production and destruction mechanisms of dust and how it evolves with metallicity and over cosmic time.

In my talk I will present my recent results on characterizing the dust depletion of 18 metals (C, P, O, Cl, Kr, S, Ge, Mg, Si, Cu, Co, Mn, Cr, Ni, Al, Ti, Zn and Fe) using relative abundances in different galactic environments, including the Milky Way, the Magellanic Clouds and damped Lyman-alpha absorbers (DLAs) towards quasars (QSOs) and towards gamma-ray bursts (GRBs). Our inferred dust depletion measurements are then used to estimate the dust-tometal ratio (DTM), dust-to-gas ratio (DTG) and the dust composition in the ISM in these different galactic environments. These results have implications on the origin of cosmic dust and the dominant processes of dust production.

Dust Masses for Normal Star-forming Galaxies as Determined with the Aid of the Dale-Helou Phenomenological Model Template Spectra

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Dust is crucial in understanding the properties and evolution of galaxies as well as the formation of stars and planets. It controls the absorption and scattering of starlight, which affects the observations of distant objects and the overall structure of galaxies. We present a novel method to estimate the dust masses for normal star-forming galaxies, utilizing the Dale-Helou Phenomenological Model Template Spectra. We derive the dust mass for each spectral template and test this method by comparing the dust masses for real galaxies with that derived from detailed dust models.

Chemical Structures of Interstellar Polycyclic Aromatic Hydrocarbons

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The so-called "unidentified" infrared emission (UIE) features at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 µm, commonly attributed to the stretching and bending vibrations of polycyclic aromatic hydrocarbon (PAH) molecules, are ubiquitously seen in a wide variety of astrophysical regions in the Milky Way and nearby galaxies as well as distant galaxies at redshifts $z \ge 4$. While PAH is a precisely defined *chemical* term (i.e., PAHs are fused benzene rings made up of C and H atoms), astronomical PAHs are not necessarily pure aromatic compounds as strictly defined by chemists. Instead, PAH molecules in astronomical environments may include ring defects, substituents, partial deuteration, partial dehydrogenation, and sometimes super-hydrogenation. Astronomical PAHs often also include an aliphatic component (e.g., aliphatic side-groups like methyl –CH₃ may be attached as functional groups to PAHs). In this talk, I will review our current understanding of the chemical structures of PAHs, with special attention paid to methylation, deuteration, super-hydrogenation, and N-, S- and Osubstitution. The high sensitivity and high spatial resolution capabilities of JWST will open up an infrared window unexplored by Spitzer and unmatched by ISO observations for gaining insight into the chemical structures of PAHs.

C_{60} cation as the carrier of the λ 9577 Å and λ 9632 Å diffuse interstellar bands

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Ever since they were first detected over 100 years ago, the mysterious diffuse interstellar bands (DIBs), a set of several hundred broad absorption features seen against distant stars in the optical and near-infrared wavelength range, largely remain unidentified. The close match, both in wavelengths and in relative strengths, recently found between the experimental absorption spectra of gas-phase buckminsterfullerene ions (C $^+_{60}$) and four DIBs at λ 9632 Å, λ 9577 Å, λ 9428 Å and λ 9365 Å (and, to a lesser degree, a weaker DIB at λ 9348 Å) suggests that C $^+_{60}$ is a promising carrier for these DIBs. However, arguments against the C_{60}^+ identification remain and are mostly concerned with the large variation in the intensity ratios of the λ 9632 Å and λ 9577 Å DIBs. We search for these DIBs in the X-shooter archival data of the European Southern Observatory's Very Large Telescope, and identify the λ 9632 Å, λ 9577 Å, λ 9428 Å and λ 9365 Å DIBs in a sample of 25 stars. While the λ 9428 Å and λ 9365 Å DIBs are too noisy to allow any reliable analysis, the λ 9632 Å and λ 9577 Å DIBs are unambiguously detected and, after correcting for telluric water vapor absorption, their correlation can be used to probe their origin. To this end, we select a subsample of nine hot, O- or B0-type stars of which the stellar Mg II contamination to the λ 9632 Å DIB is negligibly small. We find that their equivalent widths, after being normalized by reddening to eliminate their common correlation with the density of interstellar clouds, exhibit a tight, positive correlation. This supports C_{60}^+ as the carrier of the λ 9632 Å and λ 9577 Å DIBs.

A Dust Evolution Model Based on the Chemical Evolution with Gas Infall

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Dust influences the physical properties of galaxies, depending on the quantity and its size distribution. Therefore, a proper understanding of dust evolution is crucial to understand the formation and evolution of galaxies. Recently, a large amount of dust has been discovered in galaxies at very high redshifts. Surprisingly, the dust-to-stellar mass ratio of such galaxies is as large as that of nearby galaxies. This is not easy to explain by current theories of dust production and evolution in galaxies, leading to a problem known as "the dust budget crisis". To explain the dust amount in these galaxies, it is necessary to supply a tremendous amount of dust at a very early stage of the galaxy. In the series of previous studies, we established a model of dust formation and evolution based on the chemical evolution of galaxies, with a closed-box assumption. With this model, we discovered that the dust accretion in the dense interstellar matter is crucial for the dust evolution. However, as we mentioned above, there remain some unsolved problems such as the origin of huge dust amount at high redshifts. In this work, we developed an extension of the previous dust evolution model, implementing an inflow of gas from the intergalactic medium. Recently, gas infall is regarded as one of the fundamental processes in galaxy evolution. We found that even if the gas is significantly consumed to form stars, dust can grow in the interstellar matter infalling from outside of a galaxy. In such a case, the dust mass compared with the stellar mass becomes larger than that predicted from a closed-box model. Therefore, a galaxy can have a sufficient amount of dust at a young galaxy age when the stellar mass is quite small. We consider the new framework to be able to explain a broader range of physical properties and observations. We present to what could be explained and what could not by this new theoretical model compared with recent observations of high-z galaxies.

Extension of dust radiation evolution model considering dust number density in distant galaxies

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In the context of galaxy evolution, dust in galaxies has a significant effect on physical quantities such as the spectral energy distribution (SED) and star formation efficiency of galaxies. We have developed a model which includes dust in the theory of galaxy evolution, accounts for the dust evolution of galaxies by considering chemical evolution (Asano et al. 2013a,b; 2014; Nozawa et al. 2015). Furthermore, a galaxy SED model has been constructed which employs this model to compute the SED of galaxies (Nishida et al. 2022). These models reproduce the observational properties of nearby dusty galaxies and the Milky Way.

However, when we try to apply our SED model to distant galaxies (e.g., Tamura et al. 2019), some modification is necessary to reproduce their observational properties. In this work, we try to resolve the problems of current SED model and reproduce the observed SEDs of very high-redshift galaxies.

The computational cost would be enormous if the radiation per dust grain is considered. Our SED model solved this problem by adopting the mega-grain approximation for the treatment of dust scattering calculation. The molecular cloud around a young star is called a clump, which is considered to be a sphere. Since distant galaxies are considered to be compact, the density in the clumps should be higher than that of nearby galaxies. Therefore, we made the clump radius have a different dependence from the entire galaxy dependence, and by increasing the number density of dust in a clump, we were able to obtain high dust emission, the same as the observed value. This approach allows for more highly reproducible simulations.

The results suggest that distant galaxies have a higher dust number density than nearby galaxies and therefore emit more dust radiation. In the future, we will examine whether we can reproduce the observations by compacting distant galaxies into a spherical rather than a one-dimensional plane approximation. Invited talk title: Dust Extinction with Gaia BP/RP Spectra

Speaker: Gregory M. Green (Max Planck Institute for Astronomy, Heidelberg, Germany)

Abstract: The three-dimensional distribution of dust in the Milky Way is richly structured on many scales. Until the mid-2010s, this structure could only be mapped in two dimensions, as a function of angular position on the sky. Most two-dimensional maps of dust column density are based on the intensity of far-infrared dust thermal emission, which is insensitive to the distance to the dust. Large surveys of Milky Way stars have dramatically changed this picture, allowing us to map the distribution of dust in 3D. Each star serves as a probe of the integrated dust column density along a particular line of sight, out to the distance of the star. By combining information from hundreds of millions of stars, we are able to reveal the complex 3D distribution of dust in our Galaxy. In this talk, I will discuss recent developments in 3D dust mapping enabled by Gaia, a space telescope that is collecting stellar astrometry and spectrophotometry at an unprecedented scale. Gaia not only enables more precise maps of dust density throughout the Milky Way, but also allows us to trace variation in the wavelength-dependence of dust extinction throughout the Galaxy, which is - as of yet - poorly understood. Better knowledge of extinction-curve variation may give insight into the dust grain-size distribution and composition, as well as its dependence on environment.

On Precise Correction of the Milky Way Dust Extinction

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Although space measurement projects like Gaia have achieved a photometric measurement accuracy of one-thousandth, our existing extinction correction is currently limited by a 1% accuracy bottleneck. However, thanks to the millions of high-quality spectra and precise atmospheric parameters provided by LAMOST, we now have a unique opportunity to address this bottleneck in unprecedented detail. Using the accurate (err ~ 0.01 -0.03 mag) multi-band reddening for millions of stars measured by the "star-pair" technique, our research has accomplished several important objectives.

Firstly, we have corrected the systematic errors of SFD and Planck extinction maps. Secondly, we have measured the reddening coefficients for colors from far-UV to mid-IR, and obtained an empirical relationship between the reddening coefficients and temperature and extinction. Finally, we have systematically depicted the two-dimensional distribution of the extinction law (Rv) in the Milky Way, and found that it is in agreement with the molecular cloud.

Overall, our research has laid a strong foundation for future advancements in this area and has the potential to improve our understanding of the structure and properties of the Milky Way.

Interstellar Extinction and Elemental Abundances

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Elements in the interstellar medium (ISM) exist in the form of gas or dust. The interstellar extinction and elemental abundances provide crucial constraints on the composition, size, and quantity of interstellar dust. Most of the extinction modeling efforts have assumed the total (gas and dust) abundances of the dust-forming elements—known as the "interstellar abundances," "interstellar reference abundances," or "cosmic abundances"—to be solar and the gas-phase abundances to be environmentally independent. However, it remains unclear whether the solar abundances are an appropriate representation of the interstellar abundances. Meanwhile, the gas-phase abundances are known to exhibit appreciable variations with local environments.

Here we explore the viability of the abundances of B stars, the solar and protosolar abundances, and the protosolar abundances augmented by Galactic chemical enrichment (GCE) as an appropriate representation of the interstellar abundances by quantitatively examining the extinction and abundances of 10 interstellar sight lines for which both the extinction curves and the gas-phase abundances of all the major dust-forming elements (i.e., C, O, Mg, Si and Fe) have been observationally determined.

Instead of assuming a specific dust model and then fitting the observed extinction curves, for each sight line we apply the model-independent Kramers-Kronig relation, which relates the wavelength-integrated extinction to the total dust volume, to place a lower limit on the dust depletion. This, to-gether with the observationally derived gas-phase abundances, allows us to rule out the B-star, solar, and protosolar abundances as the interstellar reference standard and support the GCE-augmented protosolar abundances as a viable representation of the interstellar abundances.

Interstellar X-Ray Absorption and Scattering

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Accurate estimates of the absorption of X-rays by interstellar gas and dust are of crucial importance for the analysis and interpretation of almost all astronomical soft X-ray observations. While the X-ray absorption data computed by Wilms et al. (2000) have been extensively used by the community, they assumed a reduced interstellar abundance which is just ~70% of solar. Also, they used the self-shielding approximation to estimate the X-ray absorption of dust which ignores scattering. Therefore, the X-ray absorption data of Wilms et al. could have been substantially underestimated. Here we report the state-of-the-art interstellar X-ray absorption and scattering values, derived by making use of the state-of-the-art atomic cross sections, the state-of-the-art interstellar abundances.

FUV-IR correlation and study of diffuse Far Ultraviolet emission from Holmberg II: An *AstroSat* view

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The main source of diffuse Far Ultraviolet (FUV) emission in galaxies is the scattering of starlight by the interstellar dust grains. Dust also absorbs shorter wavelength photons (UV, optical) and re-emits in the longer wavelengths, mainly in the Mid-Infrared (MIR) and Far-Infrared (FIR) resulting in diffuse Infrared (IR) emission. These two processes of scattering and absorption are complementary and are likely to result in FUV-IR correlations. In this work, we use the FUV observations of the dwarf irregular galaxy Holmberg II, obtained with the UltraViolet Imaging Telescope (UVIT) onboard AstroSat, India's first multi wavelength space mission. With a spatial resolution of 1.2"-1.6", this is the most resolved FUV observation of the galaxy till date, at a wavelength of 154 nm. We extract diffuse FUV intensities from 50 different regions throughout the galaxy and complement these with IR observations of the same regions obtained with the Spitzer Space Telescope in 7 different IR bands in order to study the FUV-IR correlations. This enables us to determine the nature of the dust grains contributing to the diffuse emission. We further model the diffuse FUV emission for some selected regions with a 3D radiative transfer model to derive the dust geometry as well as scattering properties of the dust grains, like single scattering albedo and asymmetry factor, in the galaxy. We also try to extract the point sources and determine the fraction of diffuse emission in the galaxy.

Synergies between dust and heliosphere science from the Lunar Gateway

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The Lunar Gateway is a new astronaut's "home" in orbit around the moon that will function as a hub for the lunar landings as well as pave the way for further exploration towards Mars. It will also serve as a platform for scientific experiments. Its construction by ESA, NASA, JAXA, and CSA is foreseen to start in 2024/2025 and first opportunities for scientific experiments may be available from the early 2030s. The Gateway offers a unique platform for interstellar, interplanetary and cometary dust research due to its location at 1 AU, away from Earthly debris. At 1 AU, it also has a heliocentric orbital velocity that is ideal for interstellar dust in situ measurements (in March every year) and interstellar dust sample return (in September every year). In particular the next focusing phase of interstellar (and interplanetary) dust in the solar system in the early 2030s makes the timeframe of the Gateway for this research ideal. Moreover, the new generation of dust instrumentation offers opportunities for "active" sample return and dust trajectory reconstruction through the use of dust surface charge grids. This is crucial for distinguishing interstellar from interplanetary dust particles (for radii larger than ca. 0.2 micron) and to trace back dust origins from comet to comet for the cometary dust streams, allowing for the first time, statistical sampling of dust from different sources. This talk gives an overview of the science case of cosmic dust from the Lunar Gateway and its implications for astrophysics, planetary sciences, and heliospheric sciences.

Very small dust grains as a probe for exploring thermal properties of mesoscopic scale materials

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It is well known that interstellar dust grains have a continuous size distribution from several hundred nanometers to less than a nanometer [1]. Among those, dust grains below a few tens of nanometers are classified as Very Small Grains (VSGs). Since the number of molecules, contained in a VSG, ranges from hundreds to tens of thousands [2], the VSG is intrinsically a mesoscopic scale material. For mesoscopic grains, the finiteness of their sizes brings two major effects. One is the quantum interference effect by free electron clouds surrounding each ion of the grains. This effect is no longer negligible since the de Broglie wavelength of the electron clouds is about 10 nanometers when their temperature cools down to 10 K, which is comparable to or larger than their physical sizes. The other is the limitation to the application of physical properties deduced from bulk materials, for which infinitely small size is implicitly assumed, to the modeling of VSGs (e.g., [3]). Both effects have not been satisfactorily taken into account for modeling VSGs. In this paper, we focus on the latter.

The following three facts tell us that significant modifications from the bulk materials must be made for modeling VSGs. 1. When the Debye model is used to describe the thermal properties of a silicate grain that has size < 2 nanometers, the thermal energy of the grain becomes lower than $k_{\rm B}T$ at T < 10 K, where $k_{\rm B}$ is the Boltzmann constant, and *T* is the grain temperature. This indicates that the thermal emission from the VSG is truncated by the upper bound due to its thermal energy, and the spectrum, as a result, is significantly modified by the upper bound. Yet, nobody has shown the Spectral Energy Distribution (SED) from the VSGs at wavelengths longer than the submillimeter with the upper bound taken into account. 2. Since the possible longest wavelength of the vibrational modes is limited by their sizes, the energy of the first excitation level of phonons becomes as high as about 0.01 eV corresponding temperature of 100 K for a few nanometer grains. The Debye model is no more appropriate to describe the nature of the VSGs at such low temperatures. 3. The irregularity of the grain shapes and the possible randomness of the shapes may result in breaking the degeneracy of the energy levels of phonons, which causes distributions of energy levels to vary from grain to grain. Draine and Li (2001) [2] have taken into account the first effect. They have also taken into account the third one, the randomness of the energy level distributions.

In this paper, we model the thermal and radiative properties of the VSGs by taking into account the above three effects, and examine the SED of the thermal emission from the VSGs. Our preliminary model predicts that the VSGs emit not only in the mid-infrared wave bands while they stay at a temperature above 100 K, but also emit a significant amount of flux in the millimeter. Our result predicts a correlation between the intensity of the mid-infrared emission and the millimeter emission. Since VSGs are supposed to be misaligned against magnetic fields, these excess emissions only appear in the intensity SED and do not appear in the polarization SED.

Although there is some observational evidence of the existence of the millimeter excess emission in the dust SEDs [4][5][6], the existence is still under debate [7]. It is expected that force-coming high-precision CMB experiments may provide crucial results on this topic and open the opportunity to explore the thermal properties of mesoscopic scale materials through observations. We believe that revisiting the VSG modeling explicitly by taking into account the mesoscopic scale physics is one of the current topics which should be studied.

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Interstellar dust studies with in-situ measurements from spacecraft and observations from Earth

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The existence of interstellar dust in the solar system opens an exciting opportunity to study these particles. A unique fleet of spacecraft explores the inner heliosphere for years to come and will allow us to investigate the interstellar dust there. I will discuss these missions and possible interstellar dust observations. In addition, interstellar meteors have been searched ever since the Ulysses discoveries of interstellar dust in the solar system. New opportunities come up to search for interstellar meteors by using advanced radar and advanced analysis tools. I intend to combine space and meteor observations to investigate interstellar dust and my presentations will address the link between these different observations.

Japanese-German Cooperation in Space Science

Carsten Henselowsky

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Japan and Germany have been working together in the aerospace sector for over 40 years. Today, the Joint Space Declaration, signed between the Federal Ministry of Economic Affairs and Energy of Germany and the Cabinet Office of Japan in 2020, forms the political framework for cooperation between the two nations in the field of space travel.

While Japanese Space Agency JAXA is the main cooperation partner for German Space Center DLR, additional intensive relationships also exist on level of research institute and university level.

At Space Agency level, there is a regular exchange on the topics of Earth Observation, Space Science & Exploration, Human Spaceflight & Space Research, Space Sustainability as part of the DLR-JAXA Strategy Dialogue.

In the field of space science, the cooperation's on Hayabusa 2, GALA/JUICE, BepiColombo, as well as on future missions MMX and DESTINY⁺ are prominent examples of the successful cooperation between Japan and Germany.

Development of DESTINY⁺ Dust Analyser

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DESTINY+ Dust Analyser (DDA) is an impact ionization dust analyser for the JAXA's DES-TINY+ spacecraft for an active asteroid, Phaethon, flyby mission. DDA will reveal the bulk chemical composition of interplanetary and interstellar dust particles and Phaethon ejecta particles by obtaining TOF mass spectra of positive ions generated by hypervelocity impact of dust particles. This presentation reports the development status of DDA. The performance test of the DDA engineering model (EM) with the electrostatic dust accelerator at the University of Stuttgart shows a remarkably higher mass resolution (m/dm) compared to its precursor model, CDA onboard Cassini spacecraft. The adjustment of the mechanical/thermal/electrical interface with the spacecraft system is about to finish. Some important designs for dust detection such as the position and the movable range of the DDA sensor head have been finalized. The flight model (FM) design will be finalized after Critical Design Review (CDR) and its manufacturing will be ongoing this summer.

Extension of Empirical Zodiacal Dust Cloud Model to the Near-Infrared and Visible Wavelengths for the SPHEREx Mission

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Among several empirical zodiacal dust cloud models, that of Kelsall et al. (1998), based on the COBE/DIRBE survey, is most popular owing to wide wavelength coverage (from 1.25 to 240 μ m), well-calibrated observations, and implementation of cloud's small-scale structures. However, the original Kelsall model is limited at 10 photometric bands of COBE/DIRBE and simple inter- and extrapolations are not sufficient for spectral observations because features in the solar spectrum and interplanetary dust's reflectance are lost. SPHEREX (Spectro-Photometer for the History of the Universe, Epoch of Reionization, and Ices Explorer) is a NASA's medium-class mission to survey the whole sky at near-infrared wavelengths (0.75–5 μ m) with low spectral resolution ($\lambda/\Delta\lambda \sim 40$ –150) for about two years. We extended Kelsall's model for simulations of SPHEREX observations, focusing mainly on the scattering properties of interplanetary dust.

For the scattering phase function, we revisited inversion methods introduced in 1980s, taking into account the non-unity power-law exponent of dust radial distribution and the finite brightness integral. The reflectance of zodiacal light was synthesized by combining results from HST (Hubble Space Telescope), CIBER (Cosmic Infrared Background ExpeRiment), IRTS (InfraRed Telescope in Space), and AKARI to cover wavelengths from 0.27 to $4.6 \,\mu\text{m}$. The visible part of reflectance curve is similar to that of C-type asteroids, while the near-infrared part up to $2.5 \,\mu\text{m}$ is to that of S- or Q-type, as pointed out in previous studies. Meantime, a bump-like feature around $3.5 \,\mu\text{m}$ is prominent at longer wavelengths. We tried to reproduce it with hot, small dust particles penetrating the Solar System from the Local Interstellar Cloud.

Graphene, Fullerenes and Nanotubes in the Space

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We present a series work about carbon dust in the space, which includes the theoretical calculation of IR emission of graphene, C_{24} , and the possible detection of infrared emission of planar C_{24} , and also Fullerenes C_{60} close to the HII region candidate IRAS 17450–2759 toward Sgr B2. An absorption spectrum of carbon nanotube (CNT) in the space is also presented here. The IR emission spectrum of graphene from theoretical calculation showed unusual IR emission features at ~ 6.6, 9.8 and 20 μ m. We have placed an upper limit of ~ 5 ppm of C/H on the abundance of graphene in the diffuse ISM. Subsequently, we have searched for characteristic IR emission features of C_{24} toward the high-mass star formation region (HMSFR), Sgr B2, and detected possible IR emission from C_{24} at ~ 6.637, 9.853 and 20.050 μ m for the first time in HMSFR. Those three IR emission features are also accompanied by the characteristic IR emission of possible C_{60} . We also calculated the absorption spectrum of (5, 0) CNT, the smallest CNT, using the discrete dipole approximation, which exhibits four spectral features, peaking at ~ 0.3, 0.5, 0.9, and 2.9 μ m. The survey of C_{24} , C_{60} and C_{70} toward 16, 000 Spitzer spectra is on the way. The observation toward some planetary nebulae that had detected C_{24} or C_{70} had been done by using Purple Mountain Observatory (PMO) 13.7 m millimeter telescope.

Structural Elucidation of a 220 nm Absorption Peak in Carbonaceous Candidates for the Interstellar 217.5 nm Absorption Using UV Raman Spectroscopy

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The University of Electro-Communications, Japan

Several carbonaceous materials have been proposed as candidates for the interstellar 217.5 nm absorption, but the carbon structure responsible for this absorption has not been elucidated. To identify the structure, Raman spectra were measured for three carbonaceous materials (anthracite coal, carbonaceous mesophase, and quenched carbonaceous composite [QCC]) using visible (532 nm) and UV (224.3 nm) excitation wavelengths. Raman spectroscopy, which measures the magnitudes and intensities of frequency shifts that occur due to inelastic light scattering from the material, is a powerful tool for investigating the structures of carbon materials because of its sensitivity to local differences in the carbon bonding state. In particular, overlap of the excitation and absorption energies greatly enhances the Raman scattering efficiency of the absorbing components, which is called the resonance Raman scattering effect. Therefore, by comparing the differences in two types of Raman spectra, the causal structure of the absorption close to the observation (hereinafter, the 220 nm absorption) can be identified.

The visible Raman spectrum of anthracite shows peak shoulders near 1260 cm⁻¹, 1163 cm⁻¹, and 1415 cm⁻¹, in addition to the 1584 cm⁻¹ (G band) and 1336 cm⁻¹ (D band) peaks measured on ordinary amorphous carbon materials. On the other hand, the UV Raman spectrum shows two strong Raman peaks at 1263 cm⁻¹ and 1310 cm⁻¹, and two weak peaks in addition to the G band. The change in the UV Raman relative to the visible Raman appears in two peak intensities at 1263 cm⁻¹ and 1310 cm⁻¹, suggesting that the local carbon structure associated with these two Raman peaks caused resonant Raman scattering. In contrast, for amorphous carbon particles that do not exhibit a 220 nm absorption peak, the UV Raman spectrum shows a prominent Raman peak only in the G band, which is clearly different from that of anthracite. These findings indicate that the carbon structure related to the Raman peaks outside of the G band is related to the 220 nm absorption, and that the G-band associated with electronic π - π^* transitions is related to the slope of the UV-visible absorption spectrum.

Similar to anthracite, the visible Raman spectra of carbonaceous mesophase and QCC show weak peaks other than those in the G and D bands. Furthermore, the absorption peak positions of heattreated QCC are correlated with the disappearance of its weak Raman peaks. Thus, there is evidence that the carbon structure contributing to this weak Raman peak is related to the 220 nm absorption. In fact, conjugated double bonds have been proposed as a possible cause of the QCC absorption at 220 nm, and the weak peaks observed in the Raman spectra of the three samples are similar to the trend for the one-dimensional carbon structure. Considering that such similar local carbon structures are responsible for the absorption, it is a promising explanation for the similar absorption characteristics obtained in different candidate materials (anthracite, carbonaceous mesophase, and QCC). Mennella et al. noted the possibility that peculiar structural properties are required for the interpretation that there is a similar absorption peak in anthracite and hydrogeneted amorhous carbon, but they did not confirm this experimentally. In this poster presentation, the local carbon structure will be discussed based on the results of Raman spectroscopy.

The 2175Å Extinction Bump and the Aromatic Infrared Emission Bands

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The 2175Å extinction bump is the most pronounced spectroscopic feature on the interstellar extinction curve and has been recently detected in the early universe at redshifts $z\sim6.7$. Its carrier remains unidentified ever since its first detection by Stecher (1965) over half a century ago. In recent years, polycyclic aromatic hydrocarbons (PAHs), as a promising candidate carrier for the 2175Å extinction bump, has received widespread attention. PAHs are an important component of the interstellar medium and emit prominently a distinct set of bands at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 μ m. If PAHs are indeed the carrier of the 2175Å extinction bump, one would expect the PAH emission bands and the 2175Å extinction bump to somewhat correlate. To this end, we have performed a systematic exploration of the relation between the PAH emission bands and the 2175Å extinction bump, by examining the ultraviolet extinction (obtained by IUE) and the infrared emission (obtained by *Spitzer*) of about 40 high latitude clouds. The ultimate goal is to help unravel the carrier of the 2175Å extinction bump, a long-standing, half-century old mystery.

DFT Studies of the Electronic Transitions of PAHs and Their Implications for the 2175Å Interstellar Extinction Bump

Qi Lin¹, X.J. Yang¹, Aigen Li²

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The 2175 Å extinction bump is the most pronounced spectroscopic feature on the interstellar extinction curve. In recent years, it is often attributed to polycyclic aromatic hydrocarbon (PAH) molecules. To evaluate this attribution, we perform a systematic, computational study of the electronic transitions of over 40 PAH molecules in their anionic, neutral, cationic, and di-cationic charge states. We use density functional theory (DFT) to obtain their optimized geometries on ground state, and time-dependent DFT (TD-DFT) to calculate their electronic absorption spectra. The frequency-space implementation based on linear combinations of localized orbitals are adopted to obtain independent information for each state. Such calculations are quite computationally expensive, especially as the number of electronic transitions increases. The method used here gives the best compromise between computer time and accuracy to evaluate the band positions and strengths of the electronic transitions of PAHs near the 2175 Å extinction bump. It is found that the weighted sum of the absorption spectra of these PAH species closely resembles the 2175 Å interstellar extinction bump. We discuss the dependence of the computed bump strength on charge states. Using a real-time propagation scheme, we also compute the absorption spectra of PAHs up to 60 eV and compare them with the ultraviolet (UV) interstellar extinction curve, including the extinction bump and the far-UV rise.

Modeling Interstellar Dust Emission Based on the Physical Properties of Amorphous Materials Evolving the TLS Model

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Since most interstellar dust is composed of amorphous material, dust emission modeling based on amorphous properties is essential to constrain the chemical composition and atomic structure of amorphous dust compared with observations.

The two-level systems (TLS) model has been proposed for amorphous dust emission at long wavelengths, considering the low-energy transition between the lowest two levels caused by the disordered crystalline structure of atoms composing amorphous dust [1]. Thermal emission from amorphous dust estimated by the TLS model is one possibility of the origin for sub-millimeter/millimeter excess and anomalous microwave emission observed in interstellar space [2, 3]. The TLS model explains long wavelength observations, but there are some problems. First, the TLS model is derived based on the assumption that the energy difference between the two levels is widely distributed in amorphous dust. However, it is not a self-consistent model, assuming a local distribution in the formulation. In addition, our previous study implies that observations support a local distribution of the energy difference [4, 5]. Second, model parameters do not directly link amorphous dust properties. Therefore, deducing the dust properties is challenging even if one estimates the parameters from observations.

In this study, we estimate spectral energy distributions (SEDs) of amorphous dust by calculating absorption coefficients based on a soft-potential (SP) model, which describes low-temperature amorphous properties more universally while encompassing the TLS model [6]. The SP model assumes that atoms constituting amorphous dust are trapped in a double-well potential described by a quartic function. We calculate the polarizability of amorphous dust by solving the interaction with the electric field to obtain the absorption coefficient. Since this model calculates absorption coefficients from the first principles, it is self-consistent and connects model parameters with fundamental physical quantities of amorphous dust.

We developed a scheme to estimate dust SEDs by computing the SP model. As a result, we found that the SP model has the potential to reproduce observations more redundantly. In contrast, the conventional TLS model requires fine-tuning for model parameters to explain observed SEDs. This talk will explain the detail and differences in the dust spectra estimated from the SP and TLS models and discuss the expected impact of future studies comparing our model and observation.

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Simulating dust monomer collisions: expansion of the JKR theory

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Collisional sticking is the first process of dust aggregate growth. However, some problems prevent the dust from growing. One of the serious problems is the fragmentation of dust aggregates. When the dust aggregates collide at high velocities, which is about several tens m/s, they are broken and become fragments. The maximum collisional velocity can reach 50 m/s without turbulence (e.g., Adachi et al. 1976; Weidenschilling & Cuzzi 1993). To discuss this problem, we should understand the critical collision velocity of fragmentation, and many numerical simulations of dust aggregate collisions (e.g., Wada et al. 2007, 2008, 2009, 2013; Suyama et al. 2008, 2012).

Dust aggregates are composed of many monomers, which are submicron-sized particles. Dust growth processes have been investigated by numerical simulation studies. Numerical simulations are *N*-body simulations and calculate interactions between monomers based on the JKR theory, which is one of the contact theories. However, the JKR theory doesn't consider molecular effects such as molecular motions and deformation of monomers. It is suggested that they lead to energy dissipation at collisions and promote coalescence (Krijt et al. 2013; Tanaka et al. 2012). Therefore, the monomer interaction should be investigated including molecular physics.

We used Molecular Dynamics (MD) simulation to analyze molecular motions and performed simulations of monomers' head-on collision. We focused on the coefficient of restitution e and investigated the dependence on monomer radius (10-100 nm), impact velocity (20-150 m/s), and temperature (0-80 K). We adopted the Lennard-Jones potential as the intermolecular interaction.

We showed that the coefficient of restitution of the MD results is smaller than that of the JKR theory. The energy dissipation due to molecular motion and deformation makes the coefficient of restitution small. First, we found the coefficient of restitution increases with monomer radius. It is considered that the ratio of contact radius to monomer radius decreases with increasing monomer radius and that it causes this radius-dependence. We also found that *e* decreases for the impact velocity larger than 50 m/s. The JKR theory cannot predict decreasing *e* because it doesn't include the effect of monomer deformation, which causes significant energy dissipation. Finally, we found that *e* decreases with higher temperatures. Decreasing *e* represents the increasing energy dissipation and we confirmed that the kinetic energy of monomers was converted to the potential energy and kinetic energy of molecular random motions. The JKR theory doesn't consider these effects.

Based on our MD results, we tried to expand the JKR theory. We referred to Krijt et al. (2013) to introduce the dissipative force. First, we showed that the Krijt model cannot fit the MD results. Then, we modified their model to be of the form compression length dependent. This model can reproduce the MD results at low impact velocity, although it has insufficient energy dissipation at high impact velocity. This is because their model doesn't include energy dissipation due to monomer deformation. We consider that another force is required to reproduce decreasing e at high impact velocity.

Our results show that the sticking probability in the MD simulation is larger than that of the JKR theory. Therefore, we can expect that dust aggregates can more easily grow by direct sticking even at high collision velocity and the growth rate becomes fast.