Emerging Words 2016
Abstracts of selected proposals
(NNH16ZDA001N-EW)

Below are the abstracts of proposals selected for funding for the Emerging Worlds 2016 program. Principal Investigator (PI) name, institution, and proposal title are also included. 159 proposals were received in response to this opportunity. On December 9, 2016, 33 proposals were selected for funding.

Floss, Christine/Washington University
Microanalytical Characterization of Presolar Silicate Grains: Constraints on Grain Formation in Stellar Environments and Grain Survival in the Early Solar Nebula

Presolar silicate grains have been identified in all of the major types of extraterrestrial materials available for laboratory investigation and have provided a wealth of information about the building blocks from which our solar system originated. However, these studies have also identified existing gaps in our knowledge of the stellar environments in which these grains originated, the environments they have traversed after formation, their distribution in the early solar system, and the conditions leading to their survival or destruction in nebular and parent body environments. To address these outstanding questions, we propose here new studies on presolar silicates that will focus on a) detailed characterization of presolar silicates, including rare and new grain types; b) multi-element isotopic analyses; c) investigation of the effects of secondary processing on presolar silicate abundances and compositions; and d) investigation of the distributions of presolar silicates in different extraterrestrial materials.
Our study will provide ground-truth data for theoretical models of stellar grain condensation and nucleosynthetic processes and will provide constraints on the stellar environments in which these grains formed. Our work will also provide crucial information about the effects of secondary processing on presolar silicate grain survival in nebular and asteroidal reservoirs.
We will carry out detailed characterizations of presolar silicate (and oxide) grains in primitive meteorites using a combination of NanoSIMS, Auger spectroscopy and transmission electron microscopy (TEM). Grains will be identified through O isotopic imaging in the NanoSIMS and will subsequently be analyzed in situ with the Auger Nanoprobe to determine their elemental compositions. The Auger Nanoprobe is unique in its ability to provide compositional information on a spatial scale of several 10s of nanometers without requiring difficult sample preparation and, thus, is an ideal complement to the NanoSIMS for basic characterization of such grains. Based on this initial characterization, selected grains will be extracted and thin-sectioned using our focused ion beam (FIB) instrument, and will be examined by TEM to investigate crystallinities and internal structures. Other grains will be targeted for additional isotopic measurements (e.g., Si, Mg-Al, Fe).
The proposal team will consist of PI Christine Floss, Co-I Kevin Croat and Co-I Frank Gyngard, all at Washington University in St. Louis. In addition, we will request funding to support a graduate student, who will work on some of the proposed research.
The research we propose will allow us to understand the formation histories of individual presolar silicate (and oxide) grains and the stellar environments from which they originate. It will also help constrain the physico-chemical environments in the early solar system and on the parent bodies in which presolar grains are found. Our research thus supports the goals of NASA s Emerging Worlds Program to explore and observe the objects in the Solar System to understand how they formed and evolve , as outlined in the ROSES 2016 NRA and is, therefore, relevant to NASA s strategic objective to ascertain the content, origin, and evolution of the solar system& .

Walker, Richard/University of Maryland
Acquisition of a State-of-the-Art Multi-Collector Inductively-Coupled Plasma Mass Spectrometer

Goals and objectives: The primary goals of our work supported by the Emerging Wolds program are to constrain the timing of, and processes by which certain important early Solar System events occurred. We also seek to constrain the proportions and provenance of materials involved in these processes. Our contributions to these topics will be achieved primarily via the analysis and interpretation of siderophile element abundances and isotopic compositions. Siderophile element tools to be used include the short-lived 182Hf-182W and long-lived 187Re-187Os isotopic systems, nucleosynthetic variations in the isotopic compositions of Ru and Mo, as well as the measurement and modeling of abundances of the highly- and moderately-siderophile elements (HSE: including Re, Os, Ir, Ru, Pt, Pd; MSE: including Mo and W).

The objective of this proposal is to obtain funds to replace an existing multi-collector inductively-coupled plasma mass spectrometer (MC-ICP-MS) to support the research goals of our EW grant. The existing Nu Plasma MC-ICP-MS was purchased with funding from the University of Maryland and the NSF in 2000. This instrument was the first Nu Plasma sold in the western hemisphere and predates the advent of the Thermo-Fisher Neptune. Consequently, our instrument is one of the oldest functioning MC-ICP-MS in at least the western hemisphere. The instrument is currently reaching the end of its life cycle with considerable down time. The instrument is also significantly less capable with respect to sensitivity and maximum measurement precision than current offerings from both Nu Instruments and Thermo-Fisher.

Methodology: We will use the requested instrument for several important applications in the proposed work. First, it will be used for precise measurement of siderophile element abundances and isotopic compositions. Although some of this work is done using thermal ionization mass spectrometry, because of its greater sensitivity for W and Ru, the new ICP-MS will allow us to precisely measure the isotopic compositions of these elements extracted from silicates and small pieces of metal that cannot currently be done by TIMS.

Relevance: All of the proposed work is directed towards the stated objectives of the goals of the Emerging Worlds program which aims to understand the formation and early evolution of the Solar System , and address the question "How did the Sun s family of planets, satellites, and minor bodies form and evolve?" (page C.2-1, ROSES 2016).

Krot, Alexander/University of Hawaii at Manoa
Thermal and alteration history of the CV parent asteroid

(1) To understand the accretionary and thermal histories of the CV chondrite parent asteroid, we propose to constrain the initial 26Al/27Al ratio in this body by measuring internal 26Al-26Mg isochrons in 20 30 chondrules from the least metamorphosed CV3 chondrites, including Kaba, Y-980145, and Y-86009, by the UH Cameca ims-1280 secondary ion mass-spectrometer (SIMS). To identify other weakly metamorphosed CV3s, we will use optical and scanning electron microscopy (SEM), electron microprobe analysis (EPMA), and Raman spectroscopy. The estimated initial 26Al/27Al ratio in the CV parent asteroid will be used for its thermal modeling. Our preliminary data on the inferred initial 26Al/27Al ratios in 8 Kaba (CV3.1oxB) chondrules suggest that the initial abundance of 26Al in the CV asteroid may be enough to explain thermal metamorphism experienced by CVs, but could be too low to melt this asteroid. Variations in the inferred initial 26Al/27Al ratios in CV chondrules will be also used to understand the number of chondrule generations that accreted on the CV asteroid.
(2) To understand the alteration history of the CV asteroid, we propose to study secondary mineralization in CV3s of different petrologic subtypes using optical microscopy, SEM, EPMA, electron backscatter diffraction (EBSD), Raman spectroscopy, and focused ion beam + transmission electron microscopy (FIB+TEM). Thermodynamic modeling of the identified secondary mineral parageneses will be used to constrain physico-chemical conditions of alteration.
(3) To understand the chronology of CV alteration, we propose to study 53Mn-53Cr systematics in secondary fayalite in several weakly metamorphosed CV3oxB. The 53Mn-53Cr ages of fayalite in CV3oxB will be compared with those of kirschsteinite in the reduced CV3s and in Ca,Fe-rich silicate rims around Allende dark inclusions. To define Mn-Cr relative sensitivity factors for fayalite and kirschsteinite, we have already synthesized Mn,Cr-bearing fayalite and kirschsteinite crystals. Our preliminary data indicate that fayalite and kirschsteinite in CV chondrites formed ~3 4 Ma after CV CAIs. We will also check 55Mn/52Cr ratio in other secondary Ca-Fe-rich silicates, including hedenbergite and andradite. If their ratios are high enough for SIMS measurements of 53Mn-53Cr systematics, we will search for suitable terrestrial standards or synthesize them.
(4) To constrain O-isotope compositions of the secondary minerals (d17O and d18O) and of the fluid (D17O, and, possibly, d18O) on the CV asteroid, and to understand a role of this fluid in O-isotope exchange in anorthite and melilite in refractory inclusions and chondrules, we propose to study O-isotope compositions of andradite, anorthite, dmisteinbergite, fayalite, hedenbergite, kirschsteinite, magnetite, Na-rich melilite, nepheline, sodalite, and wollastonite in CVs by SIMS. To define instrumental mass-fractionation effects for these minerals, we will measure bulk O-isotope compositions of terrestrial minerals and evaluate whether they are suitable as standards for O-isotope measurements of the secondary minerals in CV and CK chondrites by SIMS. Our preliminary data on fayalite and magnetite in Kaba indicate that D17O of the CV fluid was ~ 1.50. To understand possible effects of metasomatic alteration on O-isotope compositions of primary minerals, we will study O-isotope compositions of plagioclase and melilite in chondrules and refractory inclusions from Kaba, Y-980145 and Y-86009. Our preliminary data indicate that plagioclase in chondrules and refractory inclusions from Kaba experienced extensive O-isotope exchange with an asteroidal fluid.
(5) To understand a possible genetic relationship between the CV and CK chondrites, we propose to study secondary mineralization in the least metamorphosed CK3s, including Watson 002, NWA 2921, 4425, and 4724, using EPMA, SEM+EBSD, and FIB+TEM and compare it with secondary mineralization in one of the most metamorphosed CV3s, Allende.

Kita, Noriko/University of Wisconsin-Madison
High Resolution Al-Mg Chronology of Chondrules and Implication to the Evolution of Protoplanetary Disk

Chondrules in primitive meteorites are considered to record chemical properties and isotope reservoirs of dust particles existed in the proto-planetary disk. By using the short-lived nuclide chronometer 26Al-26Mg (half life: 0.7 million years, Ma), formation time of most chondrule are estimated at 2-3 Ma after the formation of refractory inclusions. However, detailed systematics among Al-Mg ages chondrules in comparison to their chemical and isotope properties are not well-resolved mainly due to the limitation of analytical uncertainties in inferred ages (typically 0.2-0.5 Ma).
The goal of the study is to obtain 0.1 Ma precisions and accuracy for inferred Al-Mg ages in order to address several questions that would help us to constrain disk evolution and chondrule formation models (1) total range of chondrule formation ages in a single chondrite group, (2) time difference between FeO-rich and FeO-poor chondrules in a single chondrite group, (3) test partial melting of porphyritic chondrules from magnesium isotope ratios of olivine and pyroxene.
Chondrules are selected from multiple primitive chondrites that we have already studied in the past and are known to have minimal effects of secondary processes in the parent bodies. Selected chondrules were examined by using electron microscopies (scanning electron microscope, electron microprobe analyzer) and laser Raman spectrometry and analyzed for Al-Mg chronology by using IMS 1280 at WiscSIMS. Additional oxygen isotope analyses would be also performed for those that were not analyzed previously. We will develop method of high time resolution Al-Mg chronology with upgraded high brightness primary oxygen ion source.
We will also study O-isotope ratios of crystalline silicate in Giant Cluster IDP, which are considered to be cometary origin. The results from IDPs will be compared to those of Wild 2 particles.
The proposed research is to study chemical and isotopic properties of early solar system materials and would enhance our understanding of protoplanetary disk evolution. Therefore, it is relevant to the scope of the Emerging Worlds Program.

Garrod, Robin/University of Virginia
Simulations of Ice Processing and Complex Organic Molecule Formation in Cometary Nuclei

Cometary nuclei are perhaps the most primitive and pristine objects in the solar system; their composition is remarkably similar to that of interstellar dust-grain ices, and a number of the most complex organic molecules detected in the gas phase of star-forming cores are also detected in cometary comae. But the composition of cometary ices may be yet more chemically complex; the Stardust mission and recently the Rosetta mission both detected cometary glycine (which has not yet been found in the ISM), and many complex organic molecules have now been detected directly on the surface of comet 67P/CG by the Philae lander. Comet impacts may account for part of our planet's water, and thus may have delivered important biotic or pre-biotic compounds to the early Earth.

However, while models of complex chemical processes within organic ices in the interstellar medium are moving forward rapidly, followed by similar models of protoplanetary disk chemistry, there are no models that consider the chemistry within the cometary ices themselves - either during the "cold-storage" phase, or during the "active" phase when comets enter the inner solar system. It is postulated that the outer ice layers of Oort cloud objects undergo heavy physical and chemical processing; such may include irradiation by passing luminous stars, or by nearby supernova events. Meanwhile, numerous experiments have demonstrated the formation of amino acids in organic ices by photolysis or energetic particles. But while there are well-established models of the chemistry in the gas-phase coma, which is fed by sublimation of the nuclear ices during the active phase, the effects on the ice chemistry of the intense irradiation and heating caused by the solar approach have not been simulated in any way.

Here, it is proposed to use the PI's advanced chemical kinetics models of interstellar ice chemistry to investigate the similar processes occurring within cometary ices. By simulating both the cold-storage and active phases of cometary-ice evolution with well-established interstellar models, we may investigate to what degree the pristine ices - formed by interstellar or protoplanetary chemical activity - are further processed once comet formation has actually occurred. This processing would include the formation of the low-albedo, hydrocarbon-rich outer surface, as well as the possible formation of glycine and other complex organics relevant to life. However, the models may also highlight the destruction of those same species, if they originated in the interstellar or protoplanetary environment. The depth into the ice at which chemistry is occurring may also be important to the development and/or survival of complex organics. By adopting different physical models, differentiation between Kuiper belt/scattered-disk objects and Oort cloud objects will be possible, so that differing chemical evolutionary histories may be explored. A quantitative understanding of chemical timescales will also yield information as to the degree of chemical alteration undergone by comets that bombarded the early Earth, in comparison to recently-observed objects, and to what degree current comets really are pristine . Finally, the construction of a model for the active phase will allow the simulation of the chemistry as physical conditions change during several elliptical orbits of a comet, as the outer ice layers are ejected into the coma. These models will be the first attempt to simulate such cometary ice chemistry.

This modeling investigation is both timely and crucial for a complete understanding of important new data from the Rosetta mission and from ALMA and other observatories. It will address stated objectives of the Emerging Worlds program, specifically: "Formation of organic molecules in space"; "The chemical and physical properties of ancient materials (including asteroids and comets)"; and "The delivery of organic molecules and volatiles to planetary surfaces".

Kenyon, Scott/Smithsonian Astrophysical Observatory
The formation of Pluto's low mass satellites

We propose a comprehensive suite of numerical simulations to investigate the formation of Pluto's small satellites. This program addresses key issues in the formation, accretion, stability, and dynamical evolution of Solar System bodies throughout the history of the Solar System. We focus on the giant impact hypothesis, where a roughly Charon mass protoplanet collides with a roughly Pluto mass protoplanet. In the most popular outcome, the collision yields a binary planet surrounded by a modest cloud of debris which evolves into a set of low mass satellites. In this scenario, it is unclear whether low mass satellites can form in the debris and how they might survive tidal expansion of the binary. Our goal is to employ ORCHESTRA, our hybrid coagulation + n-body code, to address these issues. ORCHESTRA includes a multi-annulus coagulation/diffusion code and an n-body code which treats the long-term evolution of a swarm of solid particles orbiting a central mass. The central mass can be single or binary. The coagulation/diffusion code uses a statistical approach to treat physical collisions and gravitational interactions of solids and outputs the time evolution of the distributions of the number (N) and orbital parameters (a, e, and i) of particles with sizes ranging from 1 micron up to roughly 1% of the mass of the central object(s). The n-body code follows the real-time trajectories of massive particles. Massless tracer particles which respond to the changing gravitational potential of the n-bodies AND the gravitational interactions of mass bins in the coagulation code allow us to link the evolution of particles in the two codes, enabling a robust calculation of planet/satellite formation that follows all of the mass as a function of time. Our approach allows us to isolate the importance of fragmentation, gravitational stirring, migration, and the time-varying potential of the binary in the evolution of a circumbinary satellite system.

For this proposal, we plan to build on previously successful studies of the formation of small satellites in a ring surrounding a single object with the mass of Pluto-Charon (Kenyon & Bromley AJ 147:8), the migration of small satellites through debris surrounding a binary (AJ 147:8), and the expansion of a ring of debris surrounding a binary (Bromley & Kenyon, ApJ, 809:88). We will investigate the formation and orbital evolution of satellites within an expanding ring of debris surrounding an expanding binary. This study will combine the approaches used in our two previous investigations into a single theory for satellite formation. Assuming standard models for the evolution of the central binary, we will consider various initial conditions for the total mass, orbits, and the size/velocity distributions of ring material which are generally consistent with the outcomes of giant impact models (e.g., Canup AJ 141:35). Our numerical simulations will yield the masses and orbital parameters for satellites as a function of time. Comparisons of theoretical outcomes with the number and the properties of known satellites derived from Hubble Space Telescope and New Horizons observations will allow us to identify the subset of initial conditions capable of producing objects similar to the known satellites. Based on previous experience, we expect this subset to be reasonably small. Thus, our investigation will place strong constraints on giant impact models of satellite formation.

Fei, Yingwei/Carnegie Institution of Washington

Compositions, Physical Properties, and Mobility of Liquids at High Pressure: Implications for Differentiation and Core Properties of Planetary Bodies

Widespread differentiation in the early solar system is supported by extensive studies of meteorites and asteroids. Differentiation of large planetesimals (>100 km) and small planetary bodies at early stage of the planet formation is an important process to redistribute materials and energy in the interiors, leading to the formation of metallic cores. The differentiated planetesimals also have major implications for the origin of meteorite groups and histories of asteroids and planets. Differentiation certainly occurs in planetary bodies in sizes from hundreds of kilometers to Mars-size, which is the process that can be simulated in high-pressure experiments in the range of 0.1-25 GPa. One of the key questions is how the molten metal percolated through a silicate matrix to form a metallic core during the early differentiation. To address this question, we will simulate the metal-silicate separation process during the early differentiation by examining mobility of liquid metal in silicate matrix and redistribution of chemical compositions in the interior of the planetary bodies. The focus of this proposal will be (1) to examine Fe-Ni-S liquid percolation in a chondritic mantle composition (multi-phase assemblage) in the pressure range of 0.1-6 GPa, (2) to investigate percolative behavior and chemical composition of immiscible liquids in the Fe-Ni-S-O-Si-C system up to 8 GPa, and (3) to determine the change of the dihedral angle as a function of depth in the Matrian mantle. We are taking an integrated approach to study mobility and chemistry of core materials in natural compositions. The expected results will provide insights into early differentiation processes in large planetesimals and small planetary bodies and core composition of differentiated bodies in general. The proposed experiments will be conducted in the piston-cylinder and multi-anvil high-pressure devices that are used to simulate the pressure-temperature conditions of large planetesimals and small planetary bodies during differentiation. The proposed experiments are built on our experiences in high-pressure simulations and successful applications of newly developed analytical and imaging techniques to this type of research. Quantitative measurements of the percolative behavior of metallic liquid in complex natural compositions become possible only because of the development of high-resolution 3D image by using focus-ion-beam/SEM crossbeam instrument, opening a new research direction in experimental simulations of planetary processes. We have the expertise and resources to accomplish the proposed research and expect to obtain high-quality data that are fundamental for understanding the interior processes of the planetary bodies. The proposed research is within the scope of the Emerging Worlds program including (1) formation, accretion, and stability of Solar System bodies, and (2) early thermal and chemical processes occurring on small bodies regardless of whether or when they differentiated.

Dobrica, Elena/E&PS
Origins of Secondary Minerals in Interplanetary Dust Particles and Micrometeorites

This proposal aims to understand the origin of hydrated interplanetary dust particles (IDPs) and micrometeorites using detailed descriptions of the mineralogy and isotopic compositions of secondary phases. We will use electron microscopy to determine the mineral composition of secondary phases, and secondary-ion mass spectrometry to measure the O, H and Mn-Cr isotope systematics of selected phases. The proposed research will have important implications for understanding the mechanisms and formation times of secondary minerals in hydrated particles and can potentially distinguish between asteroidal and cometary alteration. Additionally, this work will provide insights into the genetic relationship between anhydrous and hydrated IDPs and micrometeorites, the Stardust cometary samples, and carbonaceous chondrites.

Science Goals and Objectives
Recently, it was postulated that ~90% of small debris particles (~10-300 µm) from the zodiacal cloud originate from the breakup of Jupiter-family comets (JFCs), and the remaining ~10% come from Oort-cloud comets and/or asteroid collisions (Nesvorný et al. 2010). However, in the interplanetary dust particles (IDP) collections, approximately half of the particles are dominated by hydrous, secondary phases (Zolensky et al. 2008) that are traditionally thought to have formed in aqueous processes on asteroids. We hypothesize that a significant fraction of these hydrated IDPs are derived from Jupiter-family comets. This hypothesis also extends to hydrated micrometeorites, which likely originate from similar parent bodies as IDPs. We will test this hypothesis by looking for variations in the petrography and isotopic composition of secondary phases in hydrated IDPs and micrometeorites that could be indicative of either an asteroidal or cometary origin. Our research, whether our hypothesis is proven or disproven, will result in a better understanding of the origin and evolution of dust in the Solar System and the effect of water on primitive bodies.

Methodology
Hydrated cometary IDPs and micrometeorites may differ from hydrated asteroidal particles in the detailed mineralogy relating to hydration processes (asteroidal aqueous alteration has been studied extensively in meteorites, we suspect cometary alteration to be somewhat different), the timing of aqueous alteration (to determine if meteorites underwent aqueous alteration at a different time than comets), and the O and H isotopic composition of secondary minerals (cometary and asteroidal water may have different O and H isotopic composition due to the presence of spatially distinct water reservoirs in the solar nebula). We will investigate the detailed mineralogy of hydrated IDPs and micrometeorites using electron-beam techniques: SEM, electron probe, and TEM at the University of New Mexico (UNM). We will measure stable (O and H) and short-lived radionuclide (Mn-Cr) isotope systems using the University of Hawaii (UH) ion probe. Handling and mounting of these small grains is challenging, but both PI Dobrica and Co-I Ogliore have many years experience handling small samples and have developed independent techniques for the preparation of IDPs and micrometeorites for ion probe and e-beam analysis.

Relevance to the Emerging Worlds Program
The Emerging Worlds program covers the physics and chemistry of events and materials that are relevant to the formation of planets, satellites, and minor bodies, including dust, and to the early history of these bodies". In particular, our proposed work with IDPs and micrometeorites directly investigates: The chemical and physical properties of ancient materials (including asteroids and comets)" as well as Studies of chemical and isotopic properties of planetary materials" as stated in C.2 Emerging Worlds of 2015 NASA-ROSES.

Garvie, Laurence/Arizona State University
Investigation of nanoprecipitates within meteoritic metals as tracers of early Solar System processes

Goals: Here is proposed a TEM- and micro-PIXE-based study of nanoprecipitate structures, compositions, and distributions within iron meteorites and iron-rich meteorites. The preliminary studies show that nanoprecipitates are the hosts for many of the trace elements in the meteorites, and revealing their distribution is important for understanding the formation and evolution of early Solar System materials. This study will also be extended to metals in bencubbinites (CB chondrites), which are primitive, metal-rich breccias closely related to CR and CH chondrites. The disparate origins and thermal histories of the metal from iron meteorites and bencubbinites will provide valuable information on nanoprecipitate formation and composition.
Introduction: Trace elements in iron meteorites are used to model crystallization processes that occured within asteroidal cores and to help elucidate the formation and thermal history of metal during nebular and planetary differentiation processes. While trace elements are determined by a number of analytical techniques such as SIMS and laser ablation ICPMS, these methods provide little data on the trace-element hosts. Studies of steels and alloys reveal that minor and trace elements often concentrate in nanoprecipitates, and there has been extensive study of their formation. Their chemistry, morphology, and distribution provides key information on a samples thermal history. Further, the role of trace elements in alloy formation, solidification, and physical properties is well documented. In contrast, there are virtually no studies of non-metal and PGE-rich nanoprecipitates in iron meteorites.
Preliminary work: I initiated a preliminary TEM-EDS-EELS study and found abundant nanoprecipitates of unusual compositions in a range of irons and a stony-iron meteorite: Odessa (IAB-MG), Butler (ungrouped), Gibeon (IVA), Canyon Diablo (IAB-MG), Deep Springs (ungrouped), Brenham (PMG-an), Henbury (IIIAB), and Gressk (IIAB). Nanoprecipitates were extracted by cutting a fresh surface followed by etching with either HNO3/methanol or liquid bromine. This surface was then coated with a thin layer of C, which was subsequently floated off the meteorite by placing the sample back in the etchant. The adhering nanoprecipitates were then studied by TEM-EDS-EELS. A wide range of nanoparticles was discovered, e.g., Pd-bearing alloys, PGE nuggets, Ge- and Ga- rich Ni phosphides, Cr-Mo nitrides, and Cr sulfides with PGEs. Composite nanoprecipitates were also found in Canyon Diablo and Odessa, including Cr-Mo nitrides with adhering caps of Pd-Sn or Fe-Ni-P particles. These composite nanoprecipitates provide information on precipitation sequence.
Proposed research: Nanoparticles will be extracted and characterized by TEM and electron-beam techniques. Given the challenges of quantifying heavy elements by EDS and EELS, I will also use the micro-PIXE at ASU for their elemental characterization. The goal is to provide information on the nanoscale phase petrology of metal systems, which has an important bearing on trace element behavior and in some cases, larger scale structural characteristics of metal-rich meteorites.
Programmatic considerations: The proposed study is designed to make significant advances in our understanding of the solid-state histories of meteorites, their formation, and accretion. By addressing problems related to processes that occurred in the early Solar System, we will provide fundamental new insights into the origin of our Solar System and its solid bodies. As such the proposed research encompasses the scope of the Emerging Worlds program designed to ... answer the fundamental science question of how the Solar System formed and evolved ... and ... conduct scientific invenstigations related to understanding the formation and early evolution of our Solar System.

Elsila, Jamie/NASA Goddard Space Flight Center

Can D/H isotope composition of polycyclic aromatic hydrocarbons be used to indicate the origin, conditions, and alteration history of carbonaceous chondrites?

Scientific Goals and Objectives: The stable isotopic compositions of organics in meteorites have been used both to assess terrestrial contamination and as a marker of organic molecule provenance (1,2). Deuterium enrichment in meteoritic organics could be a residual signal from the cold interstellar medium, an indicator of parent-body composition, or associated with primordial waters (3). However, these isotopic signatures are subject to fractionation during thermal and aqueous alteration. Soluble polycyclic aromatic hydrocarbons (PAHs) are abundant organic compounds in carbonaceous chondrites with well-preserved stable hydrogen isotope (D/H) ratios (3,4). Patterns of deuterium enrichment in these molecules may provide evidence of their formation environment as well as the influence of parent-body processes (3, 5, 6).

This work seeks to understand the relationship between D/H composition and molecular species. Specifically, this work would test up to six hypothesized reactions suggested for the production of PAHs in interstellar environments (3). The proposed work would also assess the influence of parent-body processing and composition on PAHs by measuring changes in the D/H expression of PAHs versus their alkylated derivatives for a selection of chondrites representing different groups and petrographic types (CM1/2, CM2, C2, CV3).

Methodology: In order to test our hypothesized mechanisms we will assess ring number, condensation, molecular weight, aromatization, regiochemistry, alkylation and H/C ratio for each PAH as well as measure the D/H composition. A major analytical challenge for acquiring D/H measurements is the complete separation of the complex mixture of PAHs and other species in chondrites, This challenge has hampered previous attempts to measure D/H in PAHs (7, 8). Our initial goals are then to optimize extraction methods for the quantitative recovery of PAH, and develop chromatographic methods, testing solid phases and solvent schedules as well as preparatory HPLC on model materials. We will then measure the D/H for each individual compound by GC-MS/IRMS. Given that molecular expression is likely influenced by a number of factors our final step will be to apply ordination methods to the complete data set in order to identify driving variables as well as co-variables.
Relevance: This laboratory study of the isotopic and molecular composition of aromatic compounds in carbon-rich meteorites addresses the Emerging Worlds goal of understanding the formation and early evolution of our Solar System. In particular, we address the areas of large-scale chemical and isotopic fractionation processes , formation of organic molecules in space and chemical and physical properties of ancient materials .

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Hartmann, Lee/University of Michigan
Propagating spiral waves in protoplanetary disks

This project will investigate the stability of propagating spiral waves in protoplanetary disks by carrying out three-dimensional numerical simulations. Spiral waves in protoplanetary disks are subject to resonant interactions with inertial modes. This can lead to the destabilization of the spiral waves into small, turbulent eddies, by transferring wave energy to inertial modes -- spiral wave instability. Improving upon our prior work, the proposed project will aim to study stability of the spiral waves excited by a planetary companion and to examine the effects of disk thermodynamics to the instability. The necessary code elements have been implemented in and tested with astrophysical (magneto-)hydrodynamic codes FARGO3D, Athena, and PLUTO by the team members. Using the proposed simulations, we will assess (1) how efficiently spiral waves are destabilized by the instability; (2) how mass and angular momentum transport via spiral waves change in response to the instability; and (3) how dust diffuses/collects within the turbulence produced by the instability. The results will have potential impact in understanding the mass transport and the formation of planetesimals/planets in the proto-solar nebula as well as in extrasolar protoplanetary systems.

Calvet, Nuria/University of Michigan
A comprehensive study of protoplanetary disk structure and evolution

We have started a program to apply the next generation of the D Alessio model to the interpretation of protoplanetary disks culled from populations of different ages and evolutionary stages with the goal of characterizing the conditions that drive disk evolution and lead to the formation of planets.

Our codes are the successors of the codes that calculate the structure and emission of irradiated accretion disks, with which we have already made important discoveries such as the identification of disks with gaps and the first finding of water ice. The new models calculate the structure of the dust and of the gas separately but self-consistently, and include several aspects that have not been fully taken into account before: (a) viscous dissipation as a heating agent of the gas; (b) solution of the disk structure equations to get self-consistent hydrostatic structures of gas and dust; (c) gas absorption in the transport of high energy radiation in addition to dust; (d) dust properties (mineralogy, size distributions, sublimation temperatures consistent with the chemistry, vertical and radial distribution) inferred from the modeling of the SED and/or results of numerical simulations; (e) Flexibility in the code to allow for surface density distributions of gas and of dust, including results from numerical models of turbulent, MRI-driven disks with radial drift and trapping of dust.

Here we propose to model the disks of stars still embedded in their infalling envelopes, and to include self-consistently the interaction of the disk and the envelope. We will calculate the structure of the disk around HL Tau, and in particular the location of the condensation fronts of volatiles for comparison with observations. Our modeling will provide much insight into the nature of the radial substructure in protoplanetary disks and the best representation of the early solar nebula.

Greenwood, James/Wesleyan University
Experimental simulations of chondrule formation by radiative heating of hot planetesimals

Chondrules are mm-sized spheres of igneous rock that are abundant in primitive meteorites. They have been the subject of innumerable studies over the decades because of their promise to reveal much about conditions in the early solar system that will guide planet formation theories. Instead of guiding theory, however, they have tended to plague it, because the circumstances of their formation, in particular the source of the required heat, remains unknown. Before we can claim to understand the formation of planets, including our own, we must account for the existence and properties of chondrules. Until their message is fully decoded, it cannot be integrated into a coherent model of how planets emerged from the protoplanetary disk.

Objectives: We propose to address the issue of chondrule formation by critically testing a new hypothesis (that we have recently published in the journal Icarus) that can explain all their known features. The idea is to heat the chondrules in a settled, dust-rich sub-layer of the protosolar nebula by radiation from embedded hot planetesimals. The primary heat source is 26-Al, which must be incubated for times of about 1 Myr in moderate-sized planetesimals before it is released as radiant energy from incandescent lava at their surfaces. We have shown that a model like this naturally accounts for the observed temperature range and cooling curves of the chondrules and for the time delay from CAI formation and the time frame of the events. Importantly, it makes strong, testable predictions about the heating and cooling rates of chondrules and provides a framework for understanding other aspects of their nature such as complementarity, multiple heating events, igneous rims and their formation in relatively high density, but H-poor environments. We will hire a postdoctoral researcher to conduct experiments to see if we can reproduce chondrule textures from reasonable starting materials under the thermal conditions of our model. We will conduct 1 atm experiments on chondrule analog compositions to simulate the temperature curves that our model predicts. We will make chondrule analog compositions from characterized, known minerals following established methodology. The experiments will be conducted in a Deltech 1 atm vertical tube furnace, capable of 1725 C peak temperature, equipped with a Eurotherm 9404 temperature controller that allows 16 programmable heating and cooling segments that can go as low as 0.1 C/min. This will allow us to access much of relevant temperature and time space to simulate both FeO-rich and FeO-poor chondrules. Chondrule analog materials will be size-sorted, weighed precisely, and loaded into high-purity iron capsules for FeO-poor chondrule experiments. We will be trying to reproduce the dominant chondrule types porphyritic chondrules. We will also be attempting to determine loss or gain of sodium during the heating and cooling steps of the experiments (a secondary consideration to the textures).

Relevance to NASA and NASA-ROSES2016-Emerging Worlds: The research proposed here is highly relevant to NASA s strategic goals. We are attempting to shed light on and perhaps solve one of the unexplained mysteries of cosmochemistry namely, how did the chondrules form? The symmetrical, highly constrained heating and cooling curves that our model predicts for chondrule formation can readily be tested in the laboratory. The proposed research is to understand chemical processing of gas, dust, and ice, as well as the chemical and physical properties of ancient materials, and is relevant to protoplanetary disk formation and evolution.

Fischer, Rebecca/Harvard University
Isotopic and chemical consequences of different accretion scenarios: Comparing models with observations

The compositions of the terrestrial planets were shaped by a variety of processes in the early Solar System, including accretion, core formation, and a late veneer. N-body simulations of terrestrial planet accretion provide different scenarios for how, where, and when the terrestrial planets grew. However, there has been limited work relating these simulations to the resulting planetary chemistry. We propose to incorporate models of Ru/Mo isotope systematics and Hf/W isotopic evolution into pre-existing N-body simulations, to test which of the various accretion scenarios are most realistic.

Ru is highly siderophile, such that the Ru isotopic composition of a planet's mantle is primarily controlled by late-accreted material; conversely, Mo is only moderately siderophile, so the mantle Mo isotopic composition reflects material accreted throughout the planet's formation. The Earth and meteorites lie on the same Ru-Mo isotopic trend, indicating that the Earth's main phase of accretion and its late veneer likely have the same isotopic provenance. To better understand this observational constraint, we will model the evolution of Ru and Mo isotopes in the terrestrial planets based on N-body simulations. This modeling will provide information about the spatial extent of an isotopically homogenous region in the inner disk and how it depends on the orbits of Jupiter and Saturn. This work will also allow us to make a testable prediction for the Ru/Mo isotopic composition of Mars.

The Hf-W isotopic composition of the terrestrial planets can be used to infer the timing of core formation, because lithophile 182Hf decays to siderophile 182W with a half-life of 9 Ma. This system is affected not only by a planet's mass evolution with time but also by the style of metal-silicate equilibration. For example, the fraction of metal that equilibrates and the pressure, temperature, and oxygen fugacity of equilibration can all affect Hf-W evolution. We will implement two models of Hf-W evolution: one in which the partition coefficient of W (DW) is assumed to be constant, to rapidly explore a wide range of parameter space with a large number of N-body simulations, and a complementary, self-consistent core formation model in which DW is pressure- and temperature-dependent, as observed experimentally, to target the regions of parameter space identified as most plausible by the first model. With this modeling we will be able to evaluate how a planet's style of accretion and differentiation affect its Hf-W isotopic composition, by comparing our results to the Hf/W ratio and W isotopic composition of Earth and Mars.

We will also apply our Ru-Mo and Hf-W modeling to analyze the composition of Theia, the Moon-forming impactor. The Earth and Moon have nearly identical isotopic compositions for most elements (e.g., O, Ti, W, Si, Li, Mg, K, Ca, Cr). In the canonical Moon-forming scenario, the Moon is formed primarily from Theia, raising the question of how the Earth and Moon could have such similar isotopic compositions. One possible solution is that the proto-Earth and Theia were extremely isotopically similar; here we will evaluate that possibility by modeling the Ru-Mo and Hf-W composition of the last giant impactor and the proto-Earth at the time of the impact.

The significance of this work is that it will help to clarify the origins of the terrestrial planets and Moon and how their compositions were shaped by early Solar System processes. We will be able to address the provenance of the terrestrial planets and their late veneers in particular, the delivery of volatile-rich material from the outer disk, the initial distribution of compositions in the disk, and the mechanisms of core formation and Moon formation. Our proposal is relevant to the Emerging Worlds themes "formation, accretion, and stability of Solar System bodies" and "planetary-scale events that affect global differentiation".

Brearley, Adrian/University of New Mexico

Origin and evolution of organic materials in chondritic meteorites: insights from coordinated in situ micro and nanoanalytical studies.

Organic material in chondritic meteorites has chemical, isotopic, structural, and textural characteristics that result from a complex series of processes that occurred in different astrophysical environments. These include the interstellar medium, the solar nebula and asteroidal parent bodies. Recent studies of organic material in chondrites has demonstrated that parent body processing has a significant effect on the characteristics of this organic material. In order to understand the evolution of organic material that was accreted into asteroidal parent bodies, it is essential to understand how different parent body processes may have affected organic materials under different conditions of alteration. We propose to examine the chemical, structural, isotopic, and textural characteristics of organic matter in situ in chondritic meteorites to gain a fuller understanding of the complex processes that have contributed to its formation and subsequent processing. By studying chondritic meteorites that have experienced different degrees and styles of alteration, such as CM, CR and CO carbonaceous chondrites, as well as unequilibrated ordinary chondrites, we hope to constrain the extent to which the characteristics of the organics have been established or modified from their original preaccretionary state by both aqueous alteration and thermal processing in the presence of an aqueous fluid. Our proposed research will test the hypothesis that progressive aqueous alteration on asteroidal parent bodies caused significant modification to the structure and chemistry of the organic material as a result of fluid-mineral-organic interactions and also changed the distribution and textural characteristics of this material. By studying the relationships between organic material and alteration mineralogy, we will constrain how different degrees and styles of alteration affected organic material and use this information to constrain the processes that have occurred within asteroidal parent bodies that contribute to the evolution of the organic materials. We will also test the hypothesis that organic material is sensitive to the conditions of alteration and that varying conditions (T, fO2, etc), as well as duration of alteration, are reflected in the chemistry, structure, texture, etc. of the organics.

The proposed research will utilize coordinated spectroscopic, isotopic and mineralogical micro and nanoanalytical techniques, such as SEM, STXM-based XANES, TEM, and NanoSIMS. These techniques will be used to characterize the distribution, functional group chemistry, stable isotopic composition (H, C, N), textural characteristics, and mineral-organic relationships, in situ, in samples that have been prepared using focused ion beam techniques from different components of the meteorites. These combined techniques allow data to be obtained that can be correlated at the scale of ~100 nm, allowing all but the smallest organic grains to be characterized. These observations will be made in the context of detailed, larger-scale mineralogical studies of chondritic meteorites that provide constraints on the style and degree of alteration.

The proposed research is relevant to the Emerging Worlds program, because it addresses the chemistry of materials that are relevant to the formation of planets, satellites, and minor bodies, including dust, and to the early history of these bodies. The work specifically address the chemical and physical properties of ancient materials (including asteroids and comets) and the early thermal and chemical processes occurring on small bodies, both stated areas of relevance in section C.2 Emerging Worlds of 2016 NASA-ROSES. Our proposed work falls under the categories of Laboratory studies and Studies of the chemical and isotopic properties of planetary materials which are supported under the Emerging Worlds program.

Flynn, George/SUNY College at Plattsburgh

Understanding the Solar Protoplanetary Disk by Determining the Elemental, Mineralogical, and Organic Content of Primitive Solar Nebula Particles

Interplanetary dust particles (IDPs) are collected from the Earth s stratosphere by NASA. One type, chondritic porous (CP) IDPs, never experienced significant thermal or aqueous processing, gravitational compaction or impact shock since their formation (Ishii et al., Science, 319, 447ff, 2008), which overprint or erase the record of early Solar System processes in all meteorites. CP IDPs are a unique assemblage of presolar grains, primitive organic matter, and early Solar Nebula condensates (Nguyen et al., LPSC 46, #2868, 2015). Each ~10 micron CP IDP, an aggregate of >104 grains, requires analysis at the sub-micron scale to characterize individual minerals or organic spots. We propose three related tasks using high-resolution, synchrotron-based x-ray fluorescence (XRF), x-ray absorption near-edge structure (XANES) and infrared (IR) spectroscopy, continuing Cosmochemistry and Exobiology funded characterization of primitive IDPs.

Task 1 Characterization of Organic Grain Coatings: We identified organic rims coating each sub-micron mineral grain in CP IDPs (Flynn et al., Earth, Planets & Space, 65, 1155ff, 2013), which likely aided grain sticking in the Solar Nebula. The structure implies a three-step formation sequence: 1) submicron grains condensed, 2) they were coated with a ~100 nm layer of organic matter, and, 3) the grains aggregated to form the first dust of the Solar Nebula. These rims are likely the earliest organic matter formed in our Solar System, which Ciesla and Sandford (Science, 336, 452ff, 2012) modeled to form by condensation of carbon-bearing ices on grain surfaces, irradiation, and heating. We will determine the functional groups in this organic by C-, N-, and O-XANES and near-field, mid-IR spectroscopy, allowing comparison with products predicted in the models. We will determine if S, P, K and other biologically important elements are present by XRF and, if so, determine their speciation by XANES using the Tender Energy Spatially Resolved X-ray Absorption Spectroscopy beamline, partially funded by a NASA LARS grant, at the National Synchrotron Light Source II (Brookhaven National Laboratory) and a Scanning Transmission X-ray Microscope at the Diamond synchrotron. This task addresses Emerging Worlds objectives: Formation of organic molecules in space, Chemical and physical processing of gas, dust, and ice, and delivery of organic molecules to planetary surfaces.

Task 2: Mineralogy and Element Distribution in Nebular Condensates: The presence of organic rims in CP IDPs allows identification of grains that formed before the dust aggregated. We identified carbonate grains, not predicted in most Nebula condensation models, having organic rims in CP IDPs (Flynn et al., MetSoc 2009). We will use Si-XANES to search for rare silicate minerals, e.g., tridymite and cristobalite reported in Wild 2 grains, in three CP IDPs, and XRF mapping to search for high-Ni, Fe-sulfides, thought to occur by hydrous processing, in anhydrous IDPs. Element mapping and mineral host determination will identify the host of elements including Al, Ca, Na, K, Mg and trace elements allowing a direct test of hosts predicted by condensation models, providing insights to improve the models, addressing the Emerging Worlds objective: Chemical and physical processing of gas, dust, and ice.

Task 3 Origin of GEMS: Bradley (Science, 265, 925ff, 1994) proposed glass with metal and sulfides (GEMS), common in CP IDPs, are interstellar silicates. Keller et al. (GCA, 75, 5336ff, 2011) indicated GEMS are Nebular condensates, with element/Si ratios too low to be interstellar, but Bradley suggests ~30% of Si in GEMS is silicone oil (the collection medium). Si-XANES easily distinguishes oil from GEMS, quantifying silicone oil content, resolving this question and addressing the Emerging Worlds objective: The chemical&properties of ancient materials.

Only Emerging Worlds has these specific goals within its Scope.

Goodrich, Cyrena/Planetary Science Institute

Petrologic, Oxygen and Chromium Isotope, and Ar-Ar Studies of Non-Ureilitic Materials in Polymict Ureilites: Implications for Mixing of Materials in the Early Solar System and Differentiation of an Ancient, Carbon-Rich Asteroid

Polymict ureilites are breccias representing regolith developed on and near the surface of a ureilitic asteroid. They consist mostly of clasts that are indistinguishable from main group ureilites. However, they also contain several other types of clasts, which provide a wealth of information not available in main group ureilites and can be used to address major unresolved problems in ureilite history. These include 1) feldspathic clasts that may represent crustal igneous rocks from the ureilite parent body; 2) carbonaceous chondrite-like (dark) clasts that may represent ureilite precursor materials; and 3) foreign clasts that provide information about the Solar System environment in which the ureilite parent body evolved. We will study these minor clast populations, with the following objectives:
Objective 1: To determine the petrologic and chemical properties of all indigenous igneous lithologies in polymict ureilites and determine the relationship of each lithology to main group ureilites, in order to understand the igneous evolution of the ureilite parent body.
Objective 2: To characterize the mineralogy and petrology, oxygen and chromium isotopes, and Ar-Ar ages of carbonaceous chondrite-like clasts in polymict ureilites, in order to determine whether they represent ureilite precursor materials or are foreign.
Objective 3: To characterize the mineralogy, petrology, and oxygen isotopes of all foreign clasts in polymict ureilites for comparison with known meteorite types, in order to provide information on the Solar System environment(s) in which the ureilite parent body accreted and evolved.

The overarching objective of the proposed work is to tap the information available in polymict ureilites to address major questions about ureilite history. Results will provide new insights into the chemical and isotopic compositions of the earliest Solar System materials, and the diversity of differentiation paths among Solar Sytem bodies.

The proposed work builds on extensive experience of the PI and collaborators in studying primitive meteorites through NASA-funded research programs. It focuses on major processes affecting planetesimals in the first few million years of Solar System history, and therefore is directly relevant to the goal of the Emerging Worlds program to understand "the formation and early evolution of the Solar System (ROSES 2016, Appendix C.2).

Meyer, Bradley/Clemson University
Cosmic Chemical Memory and the Building Blocks of the Solar System

Over billions of years of Galactic history, a variety of stellar nucleosynthesis processes created the nuclei heavier than hydrogen and helium found in the Solar System. Many of those nuclei were ejected from their stellar sources in the form of dust, which then cycled through the Galaxy before being incorporated into the cloud that became the Solar System. Along with gas, these dust grains, which carried many of the heavy nuclei into the Solar nebula, served as the initial building blocks of the Solar System. The processes in the early protoplanetary disk that formed planetary bodies did not completely homogenize the isotopes in the initial dust and gas building blocks of the Solar System, and primitive samples and bulk meteorites built from these incompletely mixed building blocks thus retain cosmic chemical memory" of the nucleosynthesis and Galactic chemical evolution processes responsible for those isotopes. Cosmic chemical memory shows up in Solar System samples as isotopic anomalies, that is, as deviations from the average Solar System isotopic abundances. The PI proposes in this work to compare isotopic anomalies in cosmochemical samples to calculations from models of nucleosynthesis and Galactic chemical evolution in order to constrain stellar processes, evolution of isotopic abundances in the interstellar medium, and the Solar System s initial chemical state and early evolution.

The PI will carry out this comparison by performing theoretical research and computer modeling. He will use models constructed on top of NucNet Tools and NucNet Projects, open-source, freely available computer codes he and his students have developed, to study nucleosynthesis, stellar evolution, and Galactic chemical evolution. He will compare the results of his calculations to isotopic anomalies measured in calcium-aluminum-rich inclusions, presolar grains, and bulk meteorites. Comparison between observed chemical-memory effects with those predicted by the PI's models will yield insights and constraints on the types of processes occurring in the stars, the interstellar medium, and the early Solar System. The work will be carried out by the PI and a to-be-named graduate and undergraduate student, and all computer codes developed will be released as free, open-source software or on a hubzero-based platform that will allow them to be run directly over the web.

The work will focus on the following topics. First, the PI will use the kinetic chemical condensation code he and students have written to study dust condensation in exploding stars to gain insight into the formation of dust in a variety of stellar outflows. Second, the PI will use the open-source ICE (inhomogeneous chemical evolution) code he and his students have developed to study the isotopic evolution of dust in the interstellar medium. The goal is to understand the potential correlated isotopic abundances in the carriers of elements into the early Solar System and the consequences for isotopic anomalies observed in primitive Solar System solids and bulk planetary-scale bodies. The PI will focus initially on anomalies in Ca, Ti, Cr, Mo, Ru, and Pd, which are well established by experimental work, but will extend the work to other elements as well.

The fundamental science question of research in the Emerging Worlds program is to understand how the Solar System formed and evolved . By studying the origin and history of the dust grains that carry the isotopes into the early Solar cloud and constitute the building blocks of the Sun and planetary bodies, the projects proposed by the PI will contribute to our understanding of the initial chemical state of the Solar System and how that state evolved as the earliest Solar System bodies formed. The release of generally useful open-source codes and the implementation of those codes on a hubzero-based platform will foster further collaboration among NASA-funded researchers and provide useful tools for public outreach.

Young, Edward/University of California Los Angeles
Measuring interstellar medium silicon isotope ratios across the Galaxy as a test of solar-system formation models

Objectives: The mean distributions of isotopes as functions of Galactocentric radius (RGC, distance from the Galactic center) are proxies for the extent of stellar processing and signposts for chemical variations with time in the Galaxy. Studies of isotope ratios vs. RGC therefore provide the context for interpreting the significance of solar-system stable isotope ratios. Our objective is to characterize the distribution of the three stable isotopes of silicon, 28Si, 29Si, and 30Si, in the interstellar medium across the Galaxy to provide context for interpreting the isotope ratios in pre-solar grains and the solar system as a whole. Our survey will constitute the first new systematic investigation of interstellar medium Si isotope ratios since the early 1980s (excluding cosmic rays). The results will test Galactic Chemical Evolution (GCE) models used to assess the environment in which the solar system formed.

The ratios of secondary to primary silicon isotopes in the solar system are surprisingly low compared with older pre-solar SiC grains found in meteorites. This aberration has been used as possible evidence for extraordinary enrichment of the primary isotope, 28Si, by supernovae in the region in which the Sun formed. Oxygen isotopes also hint at supernova enrichment in the form of excess 18O relative to 17O. In order to verify or contravene the idea that the birth environment of the solar system was atypical of the Galaxy 4.6 Gyr before present, we need an understanding of how relevant stable isotope ratios have evolved with time and place in the Galaxy (i.e., over the last 4.6 Gyrs). If our solar system fits with the general picture of secular variations in stable isotope ratios in the Galaxy, then it would suggest that the answer to the question of whether we are normal or not is at least in part in the affirmative. Conversely, if our solar system exhibits significant departures from the averages expected from an analysis of the distribution and evolution of isotopes in the Galaxy, then we will be impelled to search for extraordinary circumstances to explain these departures in isotopic abundances (enrichment by nearby supernovae is the most obvious example). Isotopes of silicon are thought to be an example of the latter case but a firm Galactic reference frame for interpretation of the solar data is not in place.

Approach: This proposal is to carry out an in-depth study of silicon isotope ratios in molecular clouds across the Galaxy using the Green Bank Telescope (GBT) for the 28SiO, 29SiO, and 30SiO J=1-0 transitions in the Q band (43 GHz). Our group has already collected a large fraction of the required GBT data. We require funds to support a graduate student (a student has already been assigned to the project) to process these data as part of the student s PhD project. Processing includes computing the effects the systematic errors that can arise from different continuum radiation fields on the measured isotopolouge ratios, filling in gaps in the data with more observing where necessary, and creating Galactic Chemical Evolution constraints from these data.

Relevance to EW: Our study is directed entirely at improving our understanding of the isotopic composition of the solar system at the time of its birth. Absolute isotope ratios of pre-solar grains in particular, and those of the solar system as a whole more generally, cannot be interpreted without a clear understanding of the spatial variability and temporal evolution of isotope ratios in the Galaxy. Variations in isotope ratios with Galactocentric distance provide a proxy for variations with time by analogy with metallicity. The dispersion in Si isotope ratios across the Galaxy today also affords a measure of the variations expected at a given time for comparison with the dispersion seen in pre-solar grains.

Mendybaev, Ruslan/University of Chicago
Kinetic isotopic fractionation of solar system materials as constraints on their formation and evolution: Experimental modeling.

Recent advances in analytical instrumentation have generated a large volume of high-precision isotopic data in early solar system materials. The kinetic isotopic effects measured in meteorites are particularly important as they serve as fingerprints of processes that occurred during their formation and evolution. For example, mass-dependent fractionation effects in Mg, Si and O isotopes in CAIs are considered as indicators of the evaporation in low-pressure conditions, while fractionated Li and Mg isotopes in zoned crystals from Martian meteorites and lunar samples imply the diffusion-driven elemental transport during melt crystallization. However, quantitative interpretation of such effects requires their laboratory calibration which is very limited, and the common theme of the proposed research is to provide such calibration experiments under controlled conditions close to those in natural systems. Specifically, we will concentrate on: (1) isotopic fractionation caused by evaporation of CAI-like materials in low-pressure hydrogen to address conditions required to produce large mass-dependent fractionation effects in Mg, Si and O isotopes measured in the CAI minerals; the results of the experiments will also be used to reevaluate Mg isotopic mass fractionation law , which is critical to determine excess of 26Mg due to decay of 26Al and thus for early solar system chronometry; (2) chemical fractionation of redox-sensitive REEs (Ce, Eu, Yb) and U as function of fO2 and total pressure to address the conditions required for their depletions in some FUN and FUN-like CAIs and the lack of such in most normal (non-FUN) CAIs; depletion in U by ~100× in FUN CAIs compared to normal CAIs is particularly important as it has prevented use of the Pb-Pb chronometer to measure their absolute ages; (3) chemical and isotopic zonings in the laboratory-produced olivine crystals by cooling olivine composition melt at different rates and fO2 to distinguish between chemical zoning due to a crystal growth from chemically evolving melt and zoning due to interdiffusion of Mg and Fe in olivine; the results of the experiments will be used to place constraints on cooling rates and the crystal growth rate of olivine in Martian meteorites and lunar samples. Several of the proposed topics on evaporation of CAI-like melts have been previously carried out in isothermal vacuum experiments. It is very important to expand the experimental conditions to those of low-pressure hydrogen resembling solar nebula and to include effects of crystallization during evaporation.
Experiments will be conducted in a low-pressure hydrogen (~10-4 bar) furnace that will be build, in a vacuum (<10-8 bar) furnace, and in a one-atmosphere gas-mixing furnaces. The run products will be characterized using a TESCAN LYRA3 FIB/FESEM (Focused Ion Beam / Field Emission Scanning Electron Microscope) at the University of Chicago. Isotopic composition will be measured by solution and laser-ablation ICPMS (Inductively Coupled Plasma Mass Spectrometry), and by high-precision SIMS (Secondary Ion Mass Spectrometry) at the University of Chicago, University of Washington, and UCLA. The proposed research is highly relevant to the Emerging Worlds Program, which aims to understand formation and evolution of the early Solar System materials, and falls in the scope of several themes listed in the Program (e.g., large-scale chemical and isotopic fractionation processes; chemical and physical processing of gas, dust, and ice).

Davis, Andrew/University of Chicago
The early Solar System and its precursors

The early Solar System and its precursors

Science Goals and Objectives. The general theme of the proposed work is to better understand the nature and timing of mixing and nebular processing in the early Solar System, the ultimate sources of dust in the solar nebula, stellar nucleosynthesis, and the chronology of the first few million years of Solar System history. These goals are to be accomplished by measurements of chemical and isotopic compositions of a variety of meteorite samples, such as CAIs, chondrules, IDPs, presolar grains, and differentiated meteorites. (1) There are a number of unresolved issues in early Solar System chronology, including the levels of short-lived 41Ca, 60Fe, and 92Nb. By taking advantage of the high sensitivity and selectivity of laser resonance ionization mass spectrometry (RIMS), we plan to resolve these issues through analyses of CAIs and chondrules. (2) The 182Hf-182W system has been very successful for early Solar System chronology, but nearly all previous studies have relied on high precision W isotopic measurements on bulk samples and mineral separates. We will use the high sensitivity and selectivity of RIMS to do in situ 182Hf-182W dating of CAIs and zircons from differentiated meteorites. (3) CAIs rich in hibonite contain the largest isotopic anomalies (in Ca and Ti) of any Solar System materials. We will measure the isotopic compositions of a number of elements in well-characterized hibonite by RIMS to better resolve the sources of the isotopic components that formed our Solar System. (4) There are small variations in the isotopic compositions of a number of elements (Ca, Ti, Cr, Zr, Mo, Ru, Pd, Ba, Sm, Nd, Hf, W, Os) in bulk samples of different types of meteorites; somewhat larger isotope anomalies are revealed in progressive chemical leaching experiments on primitive meteorites. The carriers of these anomalies are unknown (except for Cr), but hold information about sources and solar nebular mixing. We will map primitive meteorites and IDPs at fine spatial resolution to search for the carriers of anomalies that have been revealed in leaching experiments. (5) Presolar grains have proven to be a rich source of information about individual stars. We will study the isotopic compositions and chemical abundances of minor and trace elements in SiC, graphite, silicates, and other presolar materials, as well as search for internal heterogeneities within these grains to better understand stellar nucleosynthesis in and condensation of grains around asymptotic giant branch stars and supernovae and to understand the starting materials that collapsed to form the Solar System. (6) GEMS (glass with embedded metal and sulfides) are enigmatic objects found in IDPs that may be of interstellar origin. Their small size has precluded isotopic measurements; we will analyze them by RIMS, beginning with Fe and Mg and proceeding to lower abundance elements.

Methodology. CHILI, the Chicago Instrument for Laser Ionization, is a RIMS instrument that is designed for high useful yield, and nearly complete suppression of isobaric interferences from both monatomic and molecular ions. RIMS schemes are available for all elements listed above. Also available are sample characterization and preparation equipment: (1) a TESCAN LYRA3 FESEM-FIB equipped with EDS, WDS, and EBSD; and (2) a dust-free clean room with microscopes and a micromanipulator.

Relevance. The proposed research is highly relevant to the goals of the Emerging Worlds program, which is targeted at improving understanding of the formation and early evolution of the Solar System, and will impact many of the bulleted items listed in ROSES 2016, including: protoplanetary disk formation and evolution; large-scale chemical and isotopic fractionation processes; chemical and physical processing of dust; the bulk properties of Solar System bodies; the chemical and physical properties of ancient materials; and the origin of meteorites and meteorite groups.

Cuzzi, Jeff/Ames Research Center, NASA
Growth and redistribution of condensible materials in the protoplanetary nebula

Primitive chondrite parent bodies (asteroids) accreted over several Myr, in which time models and astronomical observations tell us the gaseous nebula itself, and the solar luminosity, evolved significantly. The extended range of radioisotope ages for primitive body formation, the contents of comet Wild 2, and new hydrodynamical theories suggest the nebula was weakly turbulent. In this environment millimeter-to-meter-size particles can grow by sticking (depending on location, composition, and collisional strength), and undergo substantial inward radial migration, before being destroyed by mutual collisions or evaporating in a warmer environment. This migration can lead to a significant redistribution of the nebula condensibles relative to the evolving gas, even prior to accretion of planetesimals. The popular concepts of minimum mass nebula and local cosmic abundance are thus seen to be of questionable validity. As drifting particles transform from solid to vapor (and back) in their new warmer locations, they change the local chemical and isotopic composition. The local surface mass density of condensibles, their size distribution and composition, and the composition of the vapor in which they reside, provide critical initial conditions for models of planetesimal formation, and thus influence the subsequent evolution to planets. These properties, and the space- and timescales on which they vary, also provide context for the properties of primitive meteorites.

We have developed a new global model of particle growth and drift, which includes several unique features. It avoids the normally unwieldy calculations required to model particle coagulation, and has been parallelized, so is quite fast. The model includes all the most recent advances in experimental constraints on sticking , plus probability distribution functions in collision velocity, which allow lucky particles to grow beyond the nominal destruction threshold. Growth is constrained only by particle strength (strongly dependent on ice/rock ratio) and nebula properties (gas density, turbulent intensity). Growth and drift occur within viscously evolving models of nebula gas disks, in which midplane and photosphere temperatures are calculated self-consistently for our computed size distributions using a new opacity model developed for this purpose. The model captures the evaporation fronts where drifting particles evaporate part of their mass. This evolution leads to radial and temporal deviations from the normally assumed local cosmic abundances of the most important materials silicates, water, and carbon relative to hydrogen and to each other.

We will add several important physical effects new gas opacities, porosity and compaction models of growing particles, radial variation of turbulent intensity, disk winds, and infall. After we implement these improvements, we will focus our particle growth and evolution code on four important, and diverse, applications: (a) The limits to growth by sticking in the presence of radial drift, for a range of different prescriptions for porous growth and compaction, which set the initial conditions for planetesimal formation models; (b) The carbon and water evaporation fronts, with implications for the chemical composition of inner and outer solar system planetesimals and ultimately of planets; (c) The depletion of the Moderately Volatile Elements (MVEs) in chondrites; and (d) The delivery of heavy oxygen isotopes, produced by UV self-shielding either in the parent cloud or in the outer nebula, to the inner solar system.

Our work will provide a protoplanetary disk frame of reference for primitive meteorite properties, including a connection to nebula timescales that is now lacking; will provide realistic initial conditions for primary accretion of planetesimals and ultimately planets in the inner and outer solar system; and will motivate experimental studies of the sticking properties of realistic materials.

McKeegan, Kevin/University of California, Los Angeles
Chronological constraints on aqueous processing and the evolution of asteroidal materials

We propose to conduct a series of investigations of the mineralogic components of chondritic meteorites that are thought to have formed on planetesimals with the goal of developing improved chronological constraints on their formation and on the overall aqueous evolution on asteroids. Our analyses are directed toward developing a better understand of the sequence and timing of major events in planetary accretion and differentiation, which is directly relevant to the goals of the Emerging Worlds solicitation to understand the formation and early evolution of the Solar System and the strategic question of learning How did the Sun s family of planets, satellites, and minor bodies form and evolve?

We will utilize chronological tools that we and others have previously developed in a coordinated approach utilizing petrography, chemistry and in situ isotopic analyses. Timescales of early geologic activity on asteroidal parent bodies of meteorites will be addressed by coupled analyses of the Mn-Cr, O-isotope, and C-isotope systems in carbonates and other secondary minerals of carbonaceous chondrites. Previous data show that different carbonate mineralogies in CI chondrites have distinct oxygen and carbon isotopic compositions suggesting an evolution of fluid compositions on the CI parent body. We have developed a method to improve the accuracy of Mn-Cr dating of carbonates and we propose to use the newest generation ion microprobe at UCLA to delineate the full range and timing of fluid evolution on the parent asteroids of CI and other select carbonaceous chondrites. We also propose to follow up intriguing hints of 60Fe activity in early-formed carbonates via SIMS analyses and resonant ionization mass spectrometry (RIMS) analyses with our collaborator Andy Davis at the University of Chicago. Al-Mg and Fe-Ni systematics will be measured in select chondrules from unequilibrated chondrites by both SIMS and RIMS to better understand the abundance and distribution of 60Fe in the early solar system.

A Planetary Major Equipment request is made for purchase of a multi-sample introduction system for our new CAMECA ims 1290 ion microprobe. The ims 1290 is the primary instrument for the research proposed here and it serves other funded and proposed NASA projects, as well projects brought to the NSF National Ion Microprobe Facility. The instrument was purchased with substantial ($4M) support from the NSF Major Research Instrumentation program, nevertheless we could only afford to outfit with the most basic single-sample introduction system. The new system will allow the storage of up to six samples in the vacuum antechamber adjacent to the analysis chamber. This will enable improvements in background levels of volatile elements and will therefore lead to higher reliability and higher efficiency of analyses, including the oxygen and carbon isotope measurements proposed here.

Levison, Harold/SwRI
Planet Formation and its Effects on Small Body Reservoirs

This proposal employs a series of state-of-the-art numerical simulations to investigate the fundamental question of why the Solar System does not have planets closer to the Sun than Mercury. Specifically, we will study three mechanisms that might be responsible for the removal of a hypothetical population of intra-Mercurial planets: 1) Volk & Gladman (2015, Ap.J.Lett., in press.) suggest that the Solar System was born with 3 or more planets in this region, which were subsequently destroyed by a violent dynamical instability. 2) Batygin & Laughlin (2015, PNAS 112, 4214) envision that planets in this region were pushed into the Sun by a swarm of collisional fragments generated during a collisional cascade caused by the migration of Jupiter (i.e. the Grand Tack). 3) We present a new idea based on our recent simulations of so-called 'pebble accretion', where planetary embryos grow by the direct accretion of submeter-sized objects. In this case, large inner planets are pushed into the Sun due to gravitational interactions with the solar nebula (i.e. Type I migration). While exciting and intriguing, as we describe in the proposal, there are issues with these ideas that can only be addressed with large-scale simulations that follow both the dynamical and collisional evolution of the planetary systems as the planets grow and evolve. We propose such simulations here in order to evaluate these hypotheses.

Burton, Aaron/NASA Johnson Space Center
Are meteoritic amino acids associated with specific minerals?

Indigenous amino acids have now been found in all of the carbonaceous chondrite groups. The abundances, as well as structural, enantiomeric and isotopic compositions of amino acids differ significantly among meteorites of different groups and petrologic types. This suggests that there is a link between parent-body conditions, mineralogy, and the synthesis and preservation of amino acids (and likely other organic molecules). However, elucidating specific causes for the observed differences in amino acid composition has proven extremely challenging because samples analyzed for amino acids have typically been much larger (>100 mg powders) than the scale at which meteorite heterogeneity is observed (sub mm-scale differences, ~ 1-mg sized sample or less). Thus, the effects of differences in mineralogy on amino acid abundances are not easily discerned. Recent advances in the sensitivity of analytical instrumentation for amino acid analysis have made possible the analysis of smaller samples, enabling a new approach to investigate the link between mineralogical context and amino acid compositions/abundances in meteorites. Through coordinated mineral separation and characterization, and highly sensitive amino acid analyses, we will investigate the relationship between meteorite mineralogy and amino acid composition. By linking amino acid data to mineralogy, we will specifically identify amino acid-bearing mineral phases in different carbonaceous meteorites. This data will allow us to answer the following questions:

-How do amino acid distributions vary with mineralogy at the sub-millimeter scale?

-Do meteorites preserve a record of where amino acids were formed?

-Are amino acid enantiomeric excesses correlated with specific mineral compositions?

Answering these questions will greatly improve our understanding of the relationship between mineralogy and amino acid formation and survival of amino acids in meteorite parent bodies and other planetary bodies in our solar system. Our interdisciplinary research team is composed of experts in meteoritic organics, petrography and cosmochemistry. In the proposed work, we will employ our combined expertise to identify correlations between amino acids and specific mineral phases. Through careful meteorite disaggregation and mineral separation, amino acid and mineralogical analyses, we will identify the mineralogical hosts of amino acids in CM meteorites of petrologic types 1/2 and 2. In our preliminary results, we found observable differences in the amino acid compositions of matrix and non-matrix components of the Murchison meteorite. We will expand on these results to determine fine-scale correlations of meteorite mineralogy and amino acid composition, allowing us to answer fundamental questions about the origins and distributions of meteoritic amino acids. These answers address the Emerging Worlds stated goals of understanding the delivery of organic molecules to planetary surfaces and understanding their abundances and preservation in accreting matter.

Nesvorny, David/Southwest Research Institute
Studies of the Origin of Dynamical Structures in the Trans-Neptunian Region

Several properties of the Solar System, including the wide radial spacing and orbital eccentricities of the giant planets, can be explained if the early Solar System evolved through a dynamical instability followed by migration of planets in the planetesimal disk. Recently, we developed the latest generation of instability/migration models, whose initial conditions are tightly linked to our expectations for planet formation in the protoplanetary nebula. These models were subsequently used to better understand the dynamical origin of the Kuiper belt, Jupiter Trojans and irregular satellites. Here we propose to continue these studies with an eye to determining how the instability/migration models can be constrained from the present Solar System architecture. Specifically, we propose to study the following two themes:

Theme 1:
The dynamical structure of the Kuiper Belt is a blueprint of Neptune's orbital history. Much of this structure can be explained if Neptune migrated, smoothly or not, over several AU, and/or if Neptune was scattered to an eccentric orbit during planetary instability. These processes, and their timescales, are key to our understanding of the Kuiper belt. Here we propose to study the dynamics of the Kuiper belt with the aim of constraining Neptune's migration and the dynamical state of the original planetesimal disk. Particular attention will be given to the origin of the scattered disk. We will also test the 5th giant planet hypothesis.

Theme 2:
It has been recently proposed that the orbital alignment of distant trans-Neptunian objects (TNOs) can be interpreted as a gravitational signature of an unseen distant planet in the Solar System (hereafter planet Nine). The studies tentatively suggested planet's mass ~10 Earth masses, a large orbit (semimajor axis a~700 AU) and significant eccentricity (e~0.6). Additional constraints on planet Nine were obtained from the Cassini radio ranging data. The observational detection of planet Nine is challenging, because the existing results do not confine planet Nine's expected position on the sky sufficiently well. Here we propose to investigate whether the properties of planet Nine can be better constrained from its gravitational influence on distant TNOs. We will also include planet Nine in a formation model to understand how the hypothesized planet would act during Kuiper belt formation, and whether it could help to explain the highly inclined orbits of some TNOs.

RELEVANCE

The proposed research is fundamental to understanding the formation and early evolution of the Solar System. This is a central theme of NASA's Strategic Goals and the Emerging Worlds program. Specifically, the NRA for the Emerging Worlds program states that the program ``aims to answer the fundamental science question of how the Solar System formed and evolved", and that the program objectives include ``formation, accretion, and

stability of Solar System bodies" and ``early dynamical evolution of the Solar System". The types of studies
that are supported include ``theoretical investigations". Here we propose theoretical investigations
of the formation and early dynamical evolution of the Kuiper belt and the planet Nine hypothesis. Both
these themes are directly relevant to the NASA Strategic Goals and Research Objectives, and to the
Emerging Worlds program in particular. Our goal is to constrain planetary formation processes and the events
that have taken place in the Solar System over its history.

Hudson, Reggie/NASA's Goddard Space Flight Center
Laboratory Studies of Redox Reactions Relevant to the Chemistry of Emerging Icy Worlds

Laboratory studies of icy interstellar and solar system materials have progressed to where given an organic molecule and extraterrestrial environmental conditions the molecule's evolution can be described with reasonable confidence. We have studied such changes for many years and published our work in papers that both explain and predict astronomical observations. In contrast to this work on organic reactions stand the relatively few laboratory studies of the conversion of volatiles, both organics and inorganics, into ions of low volatility. Some of our recent studies have included a few sulfur-containing molecules, but the chemistry of many other species remains largely unexplored, especially as relates to ions.

We now propose to extend our earlier work to examine connections between selected volatiles and stable ions known or suspected to be present on primitive bodies and present-day planets. The focus of this Emerging Worlds proposal will be oxidation-reduction (redox) chemistry in low-temperature environments. We will investigate the extent to which exposure to ionizing radiation alters solid-phase half-reactions such as CN- ---> OCN- in HCN and organic nitriles. Measurements will be made at 10 - 200 K on icy solids for conditions relevant from grains to comets, KBOs, and even Mars and its moons. Infrared spectroscopy will be our main analytical tool, aided by other methods as needed. Our compositional measurements will be made in situ at low temperatures to avoid the many ambiguities that often plague interpretations of ice chemistry based on analyses of melted samples and ejected molecules. Our work will include investigations of how radiation at keV and MeV energies influences redox reactions in solids, and we already have extensive experience with the radiation-chemical methods needed. We are especially interested in low-temperature pre-planetary chemistry and radiation-induced conversions to produce ions.

Our proposal is relevant to the Emerging Worlds Program, as the latter covers "laboratory studies" related to "Chemical and physical processing of gas, dust, and ice" and "thermal and chemical processes occurring on small bodies". Our results will help to interpret data from and direct explorations of planetary bodies of interest to present and future NASA missions.

Hiroi, Takahiro/Brown University

Effects of Physical Properties, Space Weathering, and Viewing Geometry on the Visible and Infrared Reflectance Spectra of Carbonaceous Chondrites

Carbonaceous chondrites (CCs) are one of the most primitive materials which were formed in the early solar system and did not experience any differentiation other than some degrees of thermal metamorphism. Knowledge of the heliocentric distance and size distributions of CC parent bodies will greatly contribute to our understanding of the primordial distribution and later movement of raw materials in the Solar System. For identifying such CC parent bodies, visible and infrared (VIR) reflectance spectroscopy extending to about 4 micron in wavelength is one of the most useful techniques. However, not much is known about the effect of particle size, viewing geometry, and space weathering (SW) on the VIR spectra of CCs.

In this proposed research, bidirectional VIR reflectance spectra of chips, fine (<125 micron) and coarse (125-500 micron) powders, and fine powder pellets of about 7 representative CCs (Tagish Lake, CI, CM, CV, CO, CK, and dehydrated CI/CM) will be obtained under up to 4 different phase angles of 15, 30, 45, and 60 degrees. The chip and pellet samples will also be irradiated with pulse laser to simulate SW, and their VIR spectral changes will be studied. Bidirectional reflectance spectra over the 3-micron hydration band range will be obtained by measuring each sample after heating it at 200 C in vacuum to remove the effect of adsorbed water and extrapolating the spectral change. In addition X-ray diffraction measurements will be performed on the pellet samples before and after pulse-laser irradiation to see any changes in the mineral assemblage. The obtained VIR spectra will be analyzed to derive a set of spectral parameters as indices for particle size and SW degree and their phase angle dependence. The data will also be compared with asteroid spectra taken by AKARI to demonstrate identifying their meteorite counterparts and possibly detect adsorbed water. In this manner, this study will create a valuable database and a set of key spectral parameters for identifying CC parent bodies through ground-based telescopic observations or spacecraft missions.

Our work is relevant to this program in that it will enhance understanding of primitive materials and volatiles in the formation and early evolution of the Solar System, consistent with the goals of the Emerging Worlds program and NASA s particular interest in research projects that closely support its mission of exploring the Solar System, such as OSIRIS-REx.

Charnley, Steven/NASA Goddard Space Flight Center,
Theoretical Models for the Origin of Isotopic Fractionation in Primitive Solar System Materials.

We propose to continue theoretical studies aimed at elucidating the contribution of astrochemical processes to the isotopic fractionation measured in carbonaceous meteoritic material, interplanetary dust particles (IDPs) and cometary molecules. We will study isotopic fractionation of D, ^{15}N, ^{13}C isotopes by gas-phase chemical reactions and by catalytic processes on the surfaces of dust grains. We will put a particular focus on nitrogen isotope fractionation. The proposed work will allow us to delineate isotopic fractionation processes that could account for the fractionation patterns seen in primitive Solar System materials, and identify possible correlations that can be sought in subsequent laboratory analyses and observations.

We will undertake three complementary studies:
(1) We will revisit our comprehensive multi-isotope chemical network to include grain-surface fractionation
reactions. We will also investigate new pathways to ^{15}N fractionation in light of recent theoretical studies
and observational measurements.
(2) We will calculate the fractionation ratios expected in cold prestellar cores. We will benchmark the models and chemical fractionation networks against measurements of molecular isotopic ratios in cold molecular cloud cores. These are regions with very similar physical conditions to the outer disk environment and for which a larger, and growing, sample of isotopic ratios have been determined in the last three years or so.
(3) We will perform detailed theoretical studies of the chemistry of gas and dust in the cool midplane region of gas-rich protoplanetary disks, the comet-forming region of the proto-Solar Nebula. We will incorporate the comprehensive chemical fractionation networks and astrochemistry codes, previously developed with NASA support, into a state-of-the-art protoplanetary disk chemistry code. These studies will aim to quantify the importance of cold nebular chemistry to the isotopic makeup of primitive matter. The calculated ratios in, for example, water, nitriles, amines, and other organics will also provide a point of reference for the comparison of laboratory sample analysis of extraterrestrial materials with the expected products of cold gas-grain chemistry. Observations by ground-based interferometers at mm/ submm wavelengths are now able to map molecular distributions and measure isotopic ratios in protoplanetary disks (e.g. MCW80). We will compare the model results and predictions with existing and future disk observations and with observations of isotopic ratios in cometary molecules, particularly those now being returned by the ROSINA instrument on the Rosetta spacecraft at comet 67P/ Churyumov-Gerasimenko.

In both interstellar and nebular environments, we will evaluate the maximum degree of stable-isotope enhancement or depletionpresent in specific molecular functional groups, which could have been precursor reservoirs of cometary and asteroidal material. We will seek to provide explanations of the meteoritic and IDP data and identify possible correlations that can be sought in subsequent laboratory analyses. The proposed work is therefore complementary to much previous work where the formation environments of meteoritic material have been elucidated through nucleosynthetic signatures. When completed, and the results disseminated, the results from this project should aid interpretation of the isotopic anomalies found in the meteoritic record.

The proposed research is highly relevant to the Emerging Worlds Program. as it considers studies of the protosolar disk, large-scale isotopic fractionation, chemical and physical processing of gas and ice, and

understanding the chemical and physical properties of ancient materials (such as comets and meteorites).

Simon, Justin/NASA Johnson Space Center
Protoplanetary disk evolution: constraints by microscale isotopic analyses of CAIs

The proposed research will make coordinated isotopic measurements of the Solar System s first solids to determine their formation and how efficiently they were admixed in the protosolar disk. These measurements are fundamental to understanding the astrophysical timescales and environments of protoplanetary disk evolution that ultimately led to accretion of terrestrial planets. As the disk cooled, primordial dust that condensed from nebular gas intermixed with interstellar grains. Much of this material then underwent high temperature processes such as melting and evaporation prior to forming the different types of Ca-, Al-rich refractory inclusions (CAIs), which in turn have themselves undergone high temperature processing. Because CAIs have had complicated histories, formation of the earliest nebular solids, the conditions and environments where these materials where reworked, and the timescales over which these materials were homogenized to form the building blocks of planets are poorly understood.

Through measurement of refractory element signatures, primarily Ca isotopic and REE measurements, we will unveil the origins and evolution histories of the first Solar System solids. Comparison to the isotopic signatures of more volatile elements, Mg and O, and the Ca isotope ratios and REE abundance patterns in later generation meteoritic materials, such as their rims, will allow us to trace evolution of the Solar System s starting materials. Their isotopic and chemical compositions can be used to understand the conditions present in the protoplanetary disk where they formed and potentially whether they were transported to regions of the solar nebula that were significantly different from where they originated.

We propose two tasks: In Task 1 we will measure and model mass-dependent isotopic (Ca, Mg, and O) and chemical (REE) fractionation effects to determine the relative importance of condensation, evaporation, and open system/secondary processes in a representative suite of CAIs. In Task 2, for the same samples, we will measure 48Ca, 54Cr, and 17O mass-dependent isotopic effects, in coordination with Al-Mg dating, to track how efficiently the anomalies are homogenized as the protoplanetary disk evolved. We will integrate the results with computed protoplanetary disk evolution to test current model predictions for timing, environmental conditions, and extent of disk-wide mixing within the early Solar System.

We have developed new and improved analytical NanoSIMS and micromilling-TIMS techniques capitalizing on expertise of the PI and the team to study the isotopic compositions of nebular materials. The PI will lead the integration of the analytical studies with theoretical models to advance astrophysical models for the formation of solar systems.

This proposal further seeks support for a next-generation laser ablation and multi-collector inductively coupled plasma mass spectrometry (MC-ICPMS) facility for precision stable isotope studies and chronology targeting 5-25 micrometer-scale analyses of extraterrestrial materials. Our first measurements will focus on the relatively large stable isotope effects contained in fine-grained mineralogical features contained in the Solar System s first solids, as described in this proposal. This revolutionary instrument will also enable the development of analytical techniques for a wide range of new isotopic systems. Additionally, the new facility will allow us to maintain our capability to support conventional geochronology studies that until recently were run on 25- and 29-year old TIMS instruments that have now been decommissioned. We will make this novel facility available to the cosmochemistry community and will actively encourage collaborations among our peers (please see the types of projects that would likely be conducted as outlined in the letters of support in section 13).

Clemett, Simon/ERC Inc./JETS
Evolution of Organic Matter in Astromaterials from the Microscale to Macroscale

Science Goals & Objectives: Our research are to elucidate the nature, origin, and evolution of organic matter in primitive extraterrestrial samples. This will be achieved through in situ coordinated chemical, mineralogical and isotopic mapping, at micrometer to millimeter spatial scales, of carbonaceous meteorites and interplanetary dust particles (IDPs). Primitive astromaterials contain a complex assemblage of organic species whose origins span a range of astrophysical environments from cold molecular clouds -- through the hot and turbulent solar nebula to small bodies in the solar system. Consequently, the chemical structure, isotopic composition and mineralogical associations of this organic matter constitutes a chemical record of the environments and processes that led to the formation of the Solar System.

Methodology: Over the past decade our group has pioneered coordinated investigations focused on combining chemical, mineralogical, and isotopic studies of primitive astromaterials. Microscale and/or in situ characterization of organic matter requires analytical capabilities only now possible. This research leverages the use of a newly developed microprobe two-step laser mass spectrometer (u-L2MS) capable of measuring essentially all types of organic compounds with sub-femtomole sensitivity at micron-scale spatial resolution. This will be complemented by targeted microscale analysis of soluble organics performed by Co-Is Burton and Locke in the JSC Soluble Organics in Astromaterials Laboratory (SOAL). Our organic analyses will be closely coordinated with mineralogical and textural studies of the same samples by scanning electron microscopy and transmission electron microscopy, carried out by Co-Is Thomas-Keprta and Nakamura-Messenger. Finally, these same samples will be mapped for H, C, and N isotopic compositions at sub-micrometer scales with the JSC NanoSIMS ion microprobe by Co-Is Messenger and Nguyen. The combined organic, mineralogical, and isotopic constraints will be used to delineate the formation processes and source environments and subsequent evolutionary pathways. Specific goals of this coordinated investigation include (1) determining whether organic globules and/or isotopically anomalous hotspots are chemically distinct and if so to elucidate how they were formed (2) to obtain the broad-spectrum organic nature of IDPs for the first time and to identify differences with primitive meteorites that may relate to parent body or nebular processing and (3) to relate micrometer-scale organic measurements by u-L2MS to the larger-scale organic composition of primitive meteorites by SOAL.

Relevance to Emerging Worlds : This work directly addresses the central aims of the Emerging Worlds research call, specifically: [1] chemical and physical processing of gas, dust and ice ; [2] formation of organic molecules in space, [3] the chemical and physical properties of ancient materials, and, [4] the delivery of organic molecules and volatiles to planetary surfaces, including their abundances and preservation in accreting matter, and their survival through the accretion process. Furthermore it builds upon the heritage of previous bulk organic studies by addressing the spatial distribution of organic phases in primitive materials at the micron to millimeter scales. The significance of spatial resolved organic analysis is that it can greatly expand our ability to decipher the chemical record preserved by these materials, since results can be correlated with concurrent coordinated mineralogical, textural and isotopic analysis. Preliminary work has already revealed an impressive complexity and intricacy in the distribution of organic matter within carbonaceous meteorites, providing tantalizing evidence of distinct chemical and isotopic fingerprints of pre-accretional chemical processes. The proposed research studies will focus on establishing such chemical and isotopic trends.

Nittler, Larry/Carnegie Institution of Washington
Presolar materials in the early Solar System

Presolar grains of stardust are a trace constituent of primitive meteoritical materials and provide crucial information about the starting materials of the Solar System, the astrophysical context of solar system formation, transport and processing of dust in our protoplanetary disk and planetesimal alteration during the earliest stages of planet formation. We propose three multi-technique (NanoSIMS, TEM, nanoFTIR, Raman) microanalytical studies of presolar grains in meteorites and interplanetary dust particles designed to address scientific questions of high relevance to the Emerging Worlds program. The proposed work builds on our strong prior record of presolar grain research and much of it will take advantage of a new NASA-funded high-resolution RF plasma negative O ion source for the Carnegie NanoSIMS 50L ion probe expected to be installed in early 2017. It also will benefit from collaboration with world experts in stellar evolution and nucleosynthesis theory to aid in interpretation of isotopic data. The proposed studies include: 1) Isotopic (Cr and O) and TEM characterization of 54Cr rich presolar grains to better understand their origin and that of bulk nucleosynthetic isotopic variations in planetary materials. The new plasma ion source will be crucial to identification of these grains which can then be targeted for further isotopic and TEM analysis. 2) Isotopic, mineralogical and spectroscopic characterization of presolar silicate grains. The new ion source will enable isotope measurements of key elements (Mg, Si, Ca, Fe, K, &) that have thus far been technically challenging or impossible. Moreover, we will use nanoFTIR and high-resolution electron energy loss spectroscopy to characterize the infrared spectra of individual presolar silicate grains in order to provide ground truth for remote-sensing observations of circumstellar, interstellar and cometary dust. 3) Isotopic and microstructural characterization of presolar SiC grains, and their sub-grains, in meteorites. We will take advantage of new nondestructive (Raman and SEM-EDS based) methods we have developed for identification of rare sub-populations of SiC grains. This work will provide ground-truth on the nucleosynthetic processes responsible for isotopic variability observed in planetary materials and on galactic chemical evolution processes responsible for the bulk Solar composition and provide new insights into dust condensation processes. These studies will take advantage both of the new O source (for example to measure Ti isotopes in tiny TiC and TiN subgrains) and of the exciting new CHILI instrument at the University of Chicago (to measure trace-element isotopic compositions of important elements including Mo, Zr, Ba, Nd, Fe, and Ni). We will also explore applications of a new accelerator-based SIMS instrument recently constructed at the Naval Research Laboratory.

Dauphas, Nicolas/The University of Chicago
Refractory Lithophile Element Studies of the Formation and Early Evolution of the Solar System

Objectives:

The origin of all solar system materials can be traced back to small dust grains that were present in the solar protoplanetary disk 4.567 billion years ago. These dust grains then agglomerated and were incorporated in the mix of materials that made the terrestrial planets. The elements available in a planet thus depend on the nature and processing of dust during the earliest stages of the evolution of the solar system. The chemical composition of a planet is an important parameter that determines its geological, geodynamic and biological evolution by controlling how much heat-producing elements are available to power planetary differentiation, the nature of the minerals present, and how much nutrients are available to sustain life. Some meteorites have remained largely undisturbed since their formation and as such, they provide insights into the nebular processes that controlled the compositions of planets. Despite significant progress in our understanding of these processes, several questions remain unanswered.

1. What is the cause of the observed diversity of compositions among planetary bodies?
2. To what extent were presolar isotopic signatures homogenized during solar system formation? Did several nebular reservoirs coexist without mixing?
3. Can we tie the compositions of planets to meteorites?

To address these outstanding questions, we propose to measure the isotopic compositions of refractory elements Ca, Ti and selected lanthanides (Nd, Er, and Yb) in refractory inclusions and bulk chondrites.

Methodology:

Lanthanides are a family of refractory elements that share similar chemical properties but key differences in their behaviors make them invaluable tracers of evaporation/condensation processes. Much of the work done until now has focused on the relative abundances of the lanthanides but interpretations of abundance patterns are often non-straightforward. By systematically measuring the isotopic compositions of Ca, Ti, as well as highly refractory Er, moderately refractory Nd, and more volatile Yb in planetary materials, a quantitative understanding of the nebular processes governing the fractionation of refractory lithophile elements will be developed. Novel techniques will be used to separate these elements and their isotopic compositions will be analyzed by multi-collector inductively coupled plasma mass spectrometry.

Most isotopic variations follow the laws of mass-dependent fractionation, meaning that they scale as the relative difference in mass of the isotopes involved. Departures from this rule are called isotopic anomalies and stem from incomplete mixing of the products of stellar nucleosynthesis in the solar disk. In this work, we will characterize the mass-dependent and -independent isotopic compositions of refractory inclusions and bulk meteorites. Isotopic anomalies will be analyzed to document the extent to which different elements of varying refractoriness were formed by different nucleosynthetic processes and homogenized isotopically in the early solar system.

Relevance:

The overarching theme of the proposed work is to measure the isotopic composition of several refractory lithophile elements in the solar system s earliest condensates, chondrites, and planets to evaluate the extent to which nebular reservoirs were mixed and chemically fractionated before planets were formed. It is thus relevant to NASA s strategic objectives (solicitation NNH16ZDA001N-EW), which include

Large-scale chemical and isotopic fractionation processes; chemical and physical processing of gas, dust, and ice; formation, accretion, and stability of solar system bodies (document C2 of the solicitation, page c.2-1).

Smith, Rachel/North Carolina Museum of Natural Sciences
Investigating Carbon Inheritance in the Early Solar Nebula: An Interdisciplinary Approach

SCIENCE GOALS/OBJECTIVES: This project is an interdisciplinary effort to investigate carbon inheritance in the early solar nebula. Carbon is a key prebiotic element and a major component in protoplanetary materials. Thus, understanding the evolution of carbon will help constrain the astrochemical environment of terrestrial planet formation and the production of prebiotic compounds in the early solar system. The solar system 12C/13C ratio is ~ 87, which is significantly higher than the 12C/13C of the surrounding interstellar medium (~ 69). Further, high-resolution astronomical observations toward low-mass young stellar objects (YSOs) have revealed unexpected heterogeneity in gas-phase [12C16O[/[13C16O] (heretofore, 12CO/13CO), suggesting that complex chemistry may be affecting protoplanetary carbon rather than suggested direct inheritance from the parent cloud. This project aims to explain isotopic observations toward YSOs, and achieve a comprehensive understanding of the underlying chemistry affecting early carbon reservoirs in the solar nebula through the following: (1) Observations -we will analyze high-resolution CO data of bright YSOs along a Galactic gradient, observed with the Keck telescope, and informed by archived Keck and CRIRES data. Ratios of [12CO]/[13CO] derived from the data will be interpreted in the context of 12C/13C from other carbon-based reservoirs (i.e., CO and CO2 ice) that are along the same line-of-sight, thereby enabling a direct investigation of carbon inheritance in each protoplanetary system; (2) Experiments - we will perform interstellar ice experiments to explore carbon fractionation pathways between CO and CO2 molecular reservoirs, further aiding in the interpretation of astronomical observations; and (3) Models - We will create theoretical models to help parameterize observed isotope ratios and further define the chemical pathways along each line-of-sight, tracking changes in the carbon-containing gas and ice. Our goal is to add significantly to our understanding of carbon evolution in the early solar nebula, and help put the solar system into a meaningful context with respect to other protoplanetary systems.
METHODOLOGY: High-resolution rovibrational spectra from NIRSPEC on the Keck telescope will be used to derive precise abundances for CO isotopologues, including 12C18O and 12C17O, which help constrain the analysis. Observations of massive YSOs will be led by the PI and collaborator Blake, and our customized codes will be used for data reduction and analysis of new and archival data. A set of new data will be obtained to fill in missing regions of the Galactic gradient. Archival data from the CRIRES and Keck archives will be used to help constrain 13CO abundances, which are useful for input into the models. Co-I Gudipati will lead the experiments at his JPL lab, which is equipped to explore molecular reservoirs and potential fractionation mechanisms between isotopologues of CO and CO2 in ice and gas phases under relevant interstellar conditions. The CO models led by Co-I Willacy will track gas and ice isotope chemistry in a range of systems aimed at exploring CO ice- and gas-reservoirs, using appropriate physical conditions. The models will derive molecular isotope ratios across temperature gradients identified from the spectral analyses. The entire proposal team will contribute to the science, and the PI will recruit 3 students/year to participate in defined aspects of the project.
RELEVANCE: This project is relevant to many aspects of the Emerging Worlds (EW) scope, including investigations of processes that result in a significant change to the&chemical nature of the solar system,& and addresses the relevant topics of protoplanetary disk formation and evolution (via understanding their primordial core phases), large-scale isotopic fractionation processes , and chemical processing of gas and ice . Further, our study is relevant to the EW encouragement of interdisciplinary work.