Emerging Worlds
Abstracts of selected proposals
(NNH20ZDA001N-ROSES)

Below are the abstracts of proposals selected for funding for the 2020 Emerging Worlds program. The abstracts are listed by Principal Investigator (PI) name and include institution and proposal title. One hundred twenty-nine proposals were received in response to this opportunity. On November 19, 2020, 20 proposals were selected for funding.

Partha Bera / NASA Ames Research Center
Exploration of chemical reaction mechanisms to investigate the formation of organics in meteorites

Complex organic molecules relevant to terrestrial biochemistry might have chemically originated very early in the solar system's formation. Meteorites contain evidence of that process, and occasionally bring some of these molecules to earth. Meteorite samples contain nucleic acids, amino acids, sugars, sugar derivatives, and a plethora of other organic and inorganic molecules. Some of the sugar acids extracted from meteorite samples display a D-enantiomeric excess, and amino acids display an L-enantiomeric excess. Existence of sugars in meteorite samples, and their enantiomeric excess, must be a function of their synthesis, or their alteration after synthesis. Physico-chemical reasons behind the origin, relative abundances, and the emergence of enantiomeric excess are not well understood despite investigations, because of the limitations of the available experimental procedures, and because of the lack of detailed theoretical chemical studies. We propose to explore a number of reaction mechanisms for sugar synthesis namely the formose reactions, the novel carbonyl-ene mechanism that we propose here, and radical/ionic molecule mechanisms. One of the proposed mechanisms -- the carbonyl-ene mechanism -- for the gas phase synthesis of sugars up to six carbon atoms, may explain the emergence of enantiomeric excess in sugars via asymmetric synthesis. A small amount of enantiomeric excess in favor of the D-enantiomer developed by magnetoelectronic effects in the gas phase may propagate and be enhanced in the formation of larger organic molecules via the carbonyl-ene mechanism. We will study these reaction mechanisms for the abiotic chemical formation and emergence of enantiomeric preference of sugars in meteorites, by using state-of-the-art ab initio and density functional theory (DFT) quantum chemistry methods. We will use coupled cluster theory [especially, CCSD(T)] with large basis sets to achieve chemical accuracy which is necessary to differentiate between closely competing pathways of gas-phase reactions. For larger systems up to about a hundred atoms we will use modern DFT functionals which provide accurate structures, reaction pathways, barrier heights, relative abundances, and spectroscopic properties. Furthermore, we will explore reactions in ices by extensive H2O solvation, and by using a suite of polarizable continuum models (C-PCM) specifically developed for ices. The results are expected to improve significantly our understanding about the processes of organic molecule formation, especially sugar formation, in early solar system bodies.

Alan Brandon / University Of Houston

Constraining Nucleosynthetic Components In The Solar System From Combined Measurements of Os, Mo, Ru, and Pd Isotopes

Understanding dynamics and mixing in the solar nebula, the nature of presolar components present, and origin of rocky bodies including accretion and early differentiation, is fundamental to constraining the origin of our Solar System and its early evolution. Nucleosynthetic differences are present for Ca, Ti, Cr, Ni, Sr, Zr, Mo, Ru, Pr, Pd, Ba, Nd, and Sm isotopes, indicating nebular heterogeneity at the initial stages of condensation of rocky materials. Recent evidence indicates a dichotomy in nebular isotope components between different groups of chondrites. For example, 95Mo versus 94Mo in carbonaceous chondrites (CC) show a well-defined trend that is distinct from trends for ordinary (OC), enstatite (EC), and rumurutite (collectively called the NC trend) chondrites. This result has been interpreted that the CC and NC groups were formed in different regions of the Solar System with heterogeneous distribution of presolar matter of s- and r-process isotope components. Osmium on the other hand has shown to be largely homogeneous for s- and r-process components in bulk chondrites. Most differences observed in Os isotopic compositions in bulk chondrites have been interpreted as incomplete digestion leaving behind residual s-process pre-solar grains with large isotope leverage for the distinct components. Some variations are observed in fully accessed bulk chondrites and not attributed to incomplete access of Os during digestion. In addition, nucleosynthetic heterogeneity in Os isotopes has been observed in equilibrated ureilite achondrites. This is attributed to melting in the parent body where the s- and r-process components were in distinct materials, but could also have resulted from distinctions in the materials which accreted to form the ureilite parent body. In order to examine these issues and their implications to nebular dynamics, mixing, and heterogeneity, we will perform high-precision Os isotope measurements using a newly refined multistatic technique that significantly increases external precision to better delineate subtle differences in s- and r-process components. For the first time, on the same fractions that Os is measured, we will measure Mo, Ru, and Pd isotopes to put the nucleosynthetic components observed for Os into the context of the established variability for these elements, to examine potentially additional complexities in coupled variations, and to determine if multiple s- and r-process presolar carriers were extant at nebular condensation. This will be applied to bulk OC's where data are sparse but potentially indicate differences between H and LL Group parent bodies and to bulk ureilites showing strong differences in Os isotope nucleosynthetic components. CAI's will be measured to constrain their nucleosynthetic makeup as an important reservoir of refractory elements in the first stages of nebular condensation. Leaching/residue-combustion experiments will be performed on unequilibrated CC, EC, and OC. This examines whether the s- and r-process components for Os, Mo, Ru, and Pd are from the same stellar environments between the chondrite groups or whether multiple nucleosynthetic components were dispersed in the nebula heterogeneously. This will lead to a better understanding of the earliest history of the Solar System from the seeding of nucleosynthetic components, nebular condensation, accretion into terrestrial bodies and their early differentiation. This research is consistent with the Scope of the Emerging

Worlds program. Our new data will provide transformational insights into how the Solar System formed and evolved from protoplanetary disk formation and evolution, chemical and physical processing of nebular dust, bulk properties of Solar System bodies, formation, accretion, early thermal and chemical processing, and global differentiation of Solar System bodies. Such data will also help in planning for missions that will target specific bodies in our Solar System.

Adrian Brearley / University Of New Mexico

Formation and alteration of early solar system materials: Insights from coordinated micro and nanoscale mineralogic, spectroscopic, and isotopic studies.

The research outlined in this proposal is directed towards understanding the nature and origin of a variety of components in chondritic meteorites in the context of early solar nebular and parent body evolution. The goals of the research are to unravel the complex sequence of events that produced the chemically and mineralogically diverse assemblages observed in primitive meteorites. We will carry out mineralogical, petrologic, spectroscopic, and isotopic studies using a variety of combined microbeam techniques (SEM, EPMA, FIB/TEM, NanoSIMS, SIMS, microXANES, STXM, and LA-ICPMS) to constrain the nature of primary nebular materials and understand the diversity of alteration processes that contributed to the geologic evolution of small asteroidal parent bodies. The proposed research is highly relevant to the goals of the NASA Emerging Worlds program. Our proposed studies are divided into four specific areas:
1) The nature and timing of aqueous alteration on the CR chondrite parent body by studying the mineralogical, chemical, and isotopic evolution of smooth rims on chondrules and the alteration of chondrule glass and silica in silica-bearing rims in chondrules. We will focus on characterizing smooth rims to determine if they have formed as a result of rapid replacement of silica in silica-rich igneous rims on chondrules. We will also measure the oxidation state of Fe, Cr, and V in the amorphous silicate phase in smooth rims using microXANES, as a recorder of evolving oxygen fugacity during aqueous alteration. We will also study the mechanisms of hydration and alteration of chondrule glass in type II chondrules that we have identified in several CR chondrites, as an indicator of progressive alteration and hydrogen isotopic exchange between matrix and chondrules. 2) Studies of fine-grained rims and matrix in the most minimally-altered CM lithologies currently known that we have discovered in two CM chondrites, QUE 97990 and TIL 91722. These lithologies contain unaltered chondrule glass and have evidently experienced even less alteration than the Paris CM chondrite. These samples represent a unique opportunity to study what may be the largely unaltered precursors of CM chondrites and develop an understanding of the fine-grained nebular materials that were present in the CM chondrite-forming region of the solar nebula. Using NanoSIMS we will also search for presolar silicates in fine-grained rims in these minimally-altered lithologies, in an effort to determine if their low degree of alteration has preserved delicate presolar silicate grains better than any other known CM chondrite. 3) We will carry out EPMA, microXANES, and FIB-TEM studies of CO3 chondrites to address: a) the behavior of Cr and V at the microstructural level in olivine, to understand the behavior of these elements during the earliest stages of metamorphism. This work is intended to further constrain the mechanism of the change in Cr contents in ferroan

olivines that underpin the Grossman and Brearley classification scheme for low petrologic type chondrites and b) the origin of magnetite-rich CO3 chondrites that appear to have experienced an episode of oxidation at their lowest stages of thermal metamorphism (<3.1). This group of CO3s may represent a subgroup of CO3s, which has affinities to oxidized CV3 chondrites. We will examine the effects of oxidation on their matrix materials and as well as coarser-grained components such as chondrules. 4) We will carry out EPMA, FIB-TEM, and SIMS studies of REE abundances in secondary metasomatic grossular and andradite garnets in altered CAIs in the Allende CV3 chondrite to determine if they provide a record of fluid-rock interaction and elemental mass transport. We will also measure the water content and hydrogen isotopic composition of grossular in CAIs by NanoSIMS to establish if a hydrogrossular component is present that would provide evidence of the presence of aqueous fluids on the CV3 parent body.

Julie Brisset / University Of Central Florida
Understanding icy collisions in the early outer Solar System

Since the first spacecraft close encounters with cometary nuclei in the late 90's, the characteristics of the visited objects have intrigued the scientific community as to their origin and formation processes. The low densities measured indicate "rubble-pile"-like bodies and a primitive structure that has survived since their formation in the protoplanetary disk. In addition, the first close-up pictures of a Kuiper Belt Object (KBO) by the New Horizon mission, 2014 MU69, provide us with invaluable information on the physical processes involved in early planet formation. As pristine remnants of the young Solar System, comets and KBOs can give us unique insight into the conditions and processes that led to the formation of the outer Solar System bodies we observe today, like dwarf planets such as Pluto and Eris, but also the cores of giant planets.
Analytical work and numerical simulations have been used to put forward several possible formation scenarios for comets and small KBOs, in an attempt to explain their observed structure and characteristics. Experimental work to back up these models and provide input to simulations is currently very limited: so far, most experiments on grain growth in the early stages of planet formation have been performed at room temperature with dry particles and aggregates. First experiments on ice particle collisions demonstrate an increased cohesion compared to dry dust grains, but experimental data on aggregates of ice grains or ice-dust mixtures is very scarce. As water ice is a main constituent of the Solar System beyond the snowline, its differences in collision properties compared to dry dust grains are very likely to have played a crucial role in the formation of the outer Solar System bodies and a more consistent experimental data set on icy aggregates is required.
In order to increase our understanding of the formation conditions of cometesimals, we propose to perform a combination of numerical simulations and laboratory experiments on the collision and accretion behavior of aggregates composed of mixtures of ice and dust. The proposed experiment campaign will train and refine an N-body collision code. We will also study collisions between such aggregates and a large surface, simulating collisions of aggregates on an already formed comet nucleus. We will use a step-wise approach to aggregate growth: each simulated aggregate will be composed of building blocks two orders of magnitude smaller. This method will permit a constant number of

particles to be computed during impact simulations while spanning several orders of magnitude in size. This work will study the formation processes and environment of cometary nuclei and is thus aligned with the two elements of the Emerging Worlds program: (1.1) "formation of our Solar System" and (1.2) "early evolution of our Solar System". In addition, this work addresses Objective 1.1 of the 2018 NASA Strategic Plan: "Understand the Sun, Earth, Solar System, and Universe". As it is currently believed that the potential cores of the giant planets of the Solar System accreted from cometesimals, this work is also relevant to the very early formation stages of the outer planets of the Solar System.

Michael Brown / California Institute of Technology
A key observational test of dynamical-instability models of Solar System evolution

A seemingly unmistakable feature of dynamical instability models for the dynamical evolution of the early solar system is that the source population of the Kuiper belt objects (KBOs) and the Jupiter Trojans is the same. Despite the myriad modeling and observational successes of dynamical instability models, one observational objection remains strong: the KBOs and the Trojans clearly do not have the same surface composition. While it is easy to suggest that the solution is simply that KBOs, when heated to the temperatures of Trojans, undergo changes to become Trojan-like, observations of Centaurs -- former KBOs being heated to temperatures nearly as high as the Trojans -- show no evidence for this effect. Recently, we have found previously overlooked observational evidence that potentially shows, for the first time, that heating of KBOs transforms their surfaces to look like those of Trojans: KBOs which come unusually close to the sun appear to have surfaces indistinguishable from those of Trojans. These KBOs are heated to the same temperatures as the Centaurs, but, because of their longer-term orbital stability, the total amount of heating is higher. It appears that the reason Centaur surfaces appear indistinguishable from KBO surface is simply because Centaurs do not live long enough to develop Trojan-like surface. We will explore this hypothesis in three ways. (1) We will significantly enlarge the data set of measurements of the surface properties of Centaurs and low-perihelion KBOs, allowing a robust statistical certainty about how KBOs transform when heated; (2) We will investigate the dynamical history of these objects and compare the histories of the Centaurs vs. the KBOs in order to determine which parameters account for the difference; (3) We will use our new understanding of the surface evolution of distant icy bodies to put strong upper limits on the length of time that the primordial icy Kuiper belt could have existed close to the sun, potentially strongly constraining the timing of any dynamical instability. This analysis could remove the last strong observational objection to dynamical instability models. While removing the last strong observational objection certainly does not prove the model correct, the success of dynamical instability models predicting something as seemingly unrelated as how KBO surface behave when heated would be powerful evidence for such a history of our solar system. With its emphasis on understanding the dynamical evolution of the early solar system and the processes by which the planets came to the current locations, this research is clearly relevant to the Emerging Worlds program. While astronomical catalogs will be analyzed for one of the

tasks, these are all previously released and no new data will be acquired, making this program inappropriate for Solar System Observations.

Nicolas Dauphas / University Of Chicago
Rubidium and Potassium Isotopic Studies of Volatile Element Depletion in the Early Solar System

OBJECTIVES:
A distinguishing feature in the composition of planets and asteroids is their severe depletion in moderately volatile elements such as alkali elements Na, K, and Rb relative to undifferentiated meteorites (by up to a factor of 500). These depletions, which took place very early in the evolution of the solar system, greatly influenced the evolution of planetary bodies. Indeed, they controlled (1) how much heat-producing 40K was available to power planetary differentiation and the conditions of melting (Na and K lower the melting point of rocks) and (2) the availability of K and Na to biology where they serve many critical functions. Despite significant progress in improving our understanding of the reason why alkali elements are depleted, several questions remain unanswered: 1. Do these depletions reflect incomplete condensation, partial vaporization, or both? 2. Under what conditions (temperature, oxygen fugacity, saturation) were these elements lost? 3. What was the setting for these depletion (vaporization from magma oceans, impact-generated plumes, or chondrule formation)? To address these outstanding questions, we propose to build on our previous work on the Rb isotopic compositions of the Earth and Moon to measure the isotopic composition of Rb (as well as K and the relative abundances of all alkali elements and Mn for some samples) in chondrites, HED meteorites (Vesta), SNC meteorites (Mars), and products of evaporation experiments.
APPROACH: The relative depletions of the alkali elements and the isotopic composition of K were used previously to understand why planets are depleted in moderately volatile elements, but many questions remain unanswered. In order to develop a quantitative understanding of the processes that shaped the compositions of planets, we will: 1. Measure the stable isotopic compositions of the most volatile (Rb) and the most abundant (K) multi-isotope alkali elements in chondrites, HED, and SNC meteorites. These analyses will be performed by MC-ICPMS after purification following protocols already established in our laboratories. 2. Measure the relative abundances of the alkali elements (Li, Na, K, Rb, and Cs) and Mn in the same meteorite samples using the standard addition technique. 3. Conduct evaporation experiments on alkali elements and Mn to constrain their evaporation kinetics and associated isotopic fractionations. The evaporation experiments will be performed in vacuum and gas mixing furnaces, and the Rb and K isotopic compositions of the run-products will be analyzed by MC-ICPMS and SIMS. These measurements will be complemented by high-precision analyses of alkali element and Mn abundances using MC-ICPMS. The K and Rb isotopic analyses of meteorites will allow us to compare the compositions of Earth, Mars, and Vesta with those of their building blocks. The evaporation experiments will allow us to model and test scenarios of alkali element depletion in differentiated bodies, particularly in Vesta. Its heavy K isotopic composition suggests that evaporation was at play. By more precisely defining its K isotopic composition, measuring its Rb isotopic composition, and calibrating K/Rb and Na/Mn fractionation during evaporation, we will be able to

establish the conditions of moderately volatile element depletion in Vesta, and better constrain the astrophysical setting where this took place. RELEVANCE: The objective of the proposed work is to understand why planetary materials are depleted in moderately volatile elements by measuring the isotopic compositions of Rb and K in meteorites and products of evaporation experiments aimed at characterizing the kinetics of alkali loss and Mn from silicate melts. It is thus relevant to NASAs strategic objectives (solicitation NNH20ZDA001N-EW), which include: Studies of all aspects of materials present and processes occurring in and affecting the protoplanetary disk(section C.2-1).

Rogerio Deienno / Southwest Research Institute
Planet and Planetesimal Formation in the Inner Solar System

Task 1: Mass distribution in the inner Solar System. The order of magnitude difference in mass between Earth and Mars as well as the low mass and orbital excitation of the asteroid belt represent difficult challenges for terrestrial planet formation models. Proposed solutions for these problems largely disagree in terms of the initial radial distribution of mass in the early inner Solar System. In addition, the assumed radial distribution of planetesimals and embryos by these models were shown to be unrealistic when modeling planetary growth out from planetesimals. Finally, an early giant planet instability was also shown to affect terrestrial planet formation. Here, we propose to apply well-tested giant planet instabilities during terrestrial planet formation to constrain the initial distribution of mass within the early inner Solar System that would simultaneously lead to a small Mars, low mass and dynamically excited asteroid belt. This fundamental problem has major implications for planetesimal formation and early stages of planetary accretion. Task 2: Planetesimal and binary formation. The fraction of 100-km-class equal-size binaries among dynamically cold Kuiper Belt Objects (KBOs) is potentially as high as 100%. Equal-size binary formation is thought to have occurred during formation of KBOs themselves. There is only one known ~100-km-class equal-size binary within the asteroid belt (90 Antiope). What does this mean for planetesimal and binary formation in different parts of the Solar System? Here, we will determine the survival probabilities of equal-size binaries in the inner Solar System by simulating their collisional history from formation, giant planet instability, and subsequent ~4.4 Gyr of evolution. Our results will place limits on the initial equal-size binary fraction in the inner Solar System and provide important new constraints on planetesimal formation processes and their variation with heliocentric distance. Task 3: Dynamical Models and Isotopic Constraints. Isotopic measurements suggest the Solar System building blocks were divided into two distinct reservoirs, inner Solar System Non-carbonaceous Chondrites (NC), and outer Solar System Carbonaceous Chondrites (CC). Different hypotheses have been proposed to explain this NC-CC dichotomy. 1) A rapid growth of Jupiter stopped the inward flux of outer Solar System CC material. 2) The primordial solar nebula was ring-structured with different materials confined to different rings (e.g., due to pressure bumps). 3) Thermal processing of inward drifting pebbles produced dry and reduced solids in the inner Solar System and pristine (volatile rich) material elsewhere. These hypotheses have never been tested in detail. Here we perform dynamical simulations with a code known as LIPAD to determine whether these hypotheses work, fail, or what would it take to satisfy them. The proposed work is of major importance for understanding the

earliest stages of planet formation. Relevance Statement. The proposed research is fundamental to understanding the formation and early evolution of the Solar System. The scope of the Emerging Worlds program solicits fundamental research to understanding "(2.1) Formation of our Solar System", and "(2.2) Early evolution of the Solar System". Our goal is to constrain planetary formation processes and the events that have taken place in the early Solar System. Specifically, we will use observable data related to Mars and the asteroid belt to provide constraints on the initial distribution of mass within inner Solar System (Task 1; addressing 2.1 and 2.2) and for planetesimal formation models (Task 2; addressing 2.2). We will also use up to date measurements for cosmochemical data to constraint the earliest stages of planet formation (Task 3; addressing 2.1)

Jason Dworkin, Science PI Danielle Simkus / NASA Goddard Space Flight Center
Investigating the Influence of Parent Body Aqueous Alteration on the Stable Isotopic Compositions of Meteoritic Soluble Organic Matter

Scientific Goals and Objectives: The organic contents of carbonaceous chondrite (CC) meteorites provide a record of the chemical processes and prebiotic inventory of the early Solar System. Stable isotopic analyses of meteoritic organic matter offer insights into their chemical origins, including the synthetic relationships between meteoritic organic compound classes, and the processing history of parent body asteroids. Varying isotopic ratios (´13C) for soluble organic matter (SOM) across different CC petrologic types indicate a potential relationship between degree of parent body alteration and isotopic values [1,2]. Likewise, meteoritic insoluble organic matter (IOM) shifts towards isotopically lighter compositions (i.e., towards more negative ´13C values [3-6]) with increasing degree of hydrothermal alteration, potentially partially attributable to a loss of isotopically heavy labile organic matter. We propose to use laboratory simulations of aqueous alteration followed by ´13C analyses to trace these trends within a controlled system. Previous experimental work has demonstrated that hydrothermal alteration of IOM generates a diverse suite of solvent-extractable organic compounds [5,7]; however, beyond a single study of IOM-derived acetic acid ´13C values [5], the ´13C compositions of IOM-derived aliphatic soluble organics have not been reported. As such, the influence of hydrothermal alteration on the isotopic compositions of meteoritic SOM is poorly understood and our interpretations of varying stable isotopic values observed for SOM across different CC petrologic types remains largely speculative. We propose to address this gap in our knowledge by examining the generation of SOM from alteration of the IOM and assessing the influence of this process on the stable isotopic values of both components. We will focus on carboxylic acids, aldehydes, and ketones to directly build on the previous acetic acid work and expand it to a network of related compounds to better understand parent body history. We propose to: 1) subject meteorite materials to hydrothermal alteration experiments in the laboratory; 2) extract and analyze SOM before and after the alteration experiments to measure their abundances and compound-specific stable isotopic compositions (´13C); 3) analyze the change in C elemental and isotopic composition of the IOM to observe compositional changes derived from hydrothermal processing; and 4) compare these collective results to the variations in isotopic compositions reported in the literature for meteoritic organics. This proposed work will serve as the first coordinated assessment of stable isotopic compositions of soluble

organic compounds derived from experimentally altered meteoritic samples. Methodology: Bulk meteorite samples and isolated IOM will be subjected to a range of hydrothermal conditions to mimic asteroidal parent body aqueous alteration. Our established methodologies will be used to extract, isolate, and analyze IOM, monocarboxylic acids, aldehydes, and ketones before and after processing. Relevance: Except for the enstatite chondrites, hydrothermal alteration affected all chondrite groups, but particularly the types 1 and 2 CCs, and will have modified their organic material. This process will be elucidated by exploring the chemical and isotopic link between IOM and SOM to advance our understanding of the chemical nature and early evolution of the Solar System, and provide more context for the samples to be returned by OSIRIS-REx and Hayabusa2.

References: [1] Aponte et al. (2019) MAPS 54, 415-430, [2] Simkus et al. (2019) MAPS 54, 1283-1302, [3] Yabuta et al. (2007) MAPS 42, 37-48, [4] Alexander et al. (2014) MAPS 49, 503-525, [5] Oba and Naraoka (2006) MAPS 41, 1175-1181, [6] Oba and Naraoka (2009) MAPS 44, 943-953, [7] Pizzarello et al. (2013) PNAS 110, 15614-15619.

Philipp Heck / Field Museum Of Natural History
Refractory minerals -- archives from the early Solar System

The starting materials, processes and conditions ~4.6 billion years ago defined the composition of the present-day Solar System. Meteorites of the carbonaceous chondrite classes preserve a record of these starting materials. Studying these materials can provide important insight into the compositions, processes, and physical and chemical conditions of the early Solar System. It helps us better understand the early but determining stage of the Solar System's evolution, and, hence, provides valuable knowledge about our origins. Here, we propose to study the chemical and isotopic compositions of early Solar System minerals, refractory inclusions, in the Aguas Zarcas and the Murchison CM chondrite meteorites. The recently fallen Aguas Zarcas meteorite turned out to be scientifically very important, and has shown to contain refractory inclusions, while Murchison, a scientific treasure trove on its own, is one of the best studied meteorites that will serve as an important reference. We will focus on characterizing the minerals hibonite, spinel, olivine, and corundum and measuring their triple oxygen isotope compositions (Task 1), their Mg-Al systematics (Task 2), and their helium and neon isotopic compositions (Task 3). These minerals constitute a comprehensive and representative selection of solids from the condensation sequence in the early Solar System. The chosen isotopic systems have been shown to provide valuable insight into the heterogeneity and degree of mixing (oxygen) of the solar nebula, possibly the relative chronology of the formation of these minerals (Al-Mg), and the solar cosmic-ray irradiation conditions (He, Ne) these particles were exposed to. In addition, we will use state-of-the art modelling (Task 4) to address transport of particles in the solar nebula to better estimate the SCR irradiation times. The proposed work builds directly on previous published work by the team and also on the important body of knowledge on refractory inclusions acquired by the scientific community. We have demonstrated through peer-reviewed work that the proposed

methods are all feasible. All samples are already with the team, and the senior team members are experts in the respective methods. Analyzing this comprehensive suite of early Solar System condensates from Murchison and Aguas Zarcas as proposed and feeding the data to a physical model will provide new insights into the conditions of the early Solar System and are novel aspects. The work is relevant to the NASA Emerging Worlds program and would provide new, important insight into the early and defining evolution of our Solar System.

Truell Hyde / Baylor University
Experimental and numerical study of the formation of chondrule dust rims

The fine-grained dust rims (FGRs) formed around chondrules encode crucial information about how asteroids formed. Unfortunately despite both laboratory and theoretical studies, the FGR formation mechanism is still poorly understood. This project proposes a coordinated set of laboratory experiments and numerical simulations designed to better constrain the question: Did FGRs form (1) through adhesion of dust on the central object via slow speed collisions, (2) through higher-speed interactions between the dust and the object or (3) through some combination of these? This is an important question given that the majority of current theories suggest that FGRs form through slow speed collisions / adhesion of dust onto the central object with subsequent compression by the parent body. However, it is difficult for these theories to explain much of the observed data in hand. As such, it has recently been posited [1] that FGRs may form through higher speed interactions between the dust and the object producing abrasion and subsequent lower speed interactions and vacuum adhesion of dust particle fragments to the FGR. Differentiation of the two scenarios described requires an integrated experimental / numerical approach. This will be accomplished through the following goal. I. GOAL: The proposed project will experimentally explore the interaction between micron-sized dust particles and millimeter-sized chondrule analogs to better constrain FGR formation on specific surfaces. Dust structure formation on chondrule analogs and other representative surfaces will then be compared to current lab observations of collected FGR samples and numerical simulations of FGR formation. II. APPROACH AND METHODOLOGY: The goals above will be achieved employing existing experimental facilities and numerical simulations within the Center for Astrophysics, Space Physics and Engineering Research (CASPER) at Baylor University. The following experimental facilities within CASPER will be employed -- An inductively-heated plasma generator (IPG6-B) which will be used for gas wind tunnel tests in the pressure range 10 -- 100 Pa. A light gas gun (LGG) which will allow impact studies of dust onto chondrule analogs at speeds up to 1 km/s across various pressure regimes. Three GEC refence cells which will allow examination of dust-chondrule collisions at low speeds (10 m/s or less) and very low gas pressures. High-speed imaging of both particles and surfaces during the experiment as well as examination of the surfaces before and after exposition using microscopy will be provided. Each of the devices will be operated employing helium gas, since hydrogen has a significantly higher operating cost and requires specific safety precautions. Numerical simulation will be provided using a discrete-element code developed within CASPER called Aggregate_Builder (AB). AB has been used extensively to model dust coagulation. In this case, AB will be used to simulate dust

accretion onto chondrule and FGR surfaces over a range of collision velocities. This data will be matched to experimental data obtained and then used to scalethese results to other parameter regimes of interest.III. SIGNIFICANCE: The proposed work directly supports the scope of EW by addressing system processes occurring in protoplanetary disk formation. In addition to FGR formation, data obtained will inform processes leading to formation of other early solar system material. The parameter regimes examined will also allow emulation of various high-pressure regions within the solar nebula, e.g., pressure bumps, shock fronts or gap edges opened by a proto-Jupiter. Thus, this experimental / numerical investigation will provide much-needed data to researchers studying FGR and chondrite structures, as well as those interested in dust dynamics within protoplanetary disks.

[1] Liffman, Geochim. Cosmochim. Acta, vol. 264, pp. 118; 129, 2019

Colin Jackson / Tulane University, New Orleans
A combined chemical and physical investigation of metal-silicate reactions in magma oceans

Core formation dictates the initial distribution of elements within planetary interiors and is therefore a major component in setting the initial conditions of terrestrial worlds. Core formation primarily occurs during periods of magma ocean within terrestrial bodies, or periods of wide-scale melting of planets induced by energy released in the aftermath of large impacts during accretion. Here, metal from the core of the impactor sinks through the magma ocean on its way to the center of the impacted planet. As this metal descends, it chemically reacts with the surrounding magma, stripping the silicate portion of the planet of siderophile (iron-loving) elements while leaving lithophile elements behind. A major hurdle to accurately modeling core formation is that it is a coupled problem, with interrelated physical and chemical phenomena occurring under conditions that push the limits of current computational and experimental abilities. We propose a coordinated effort to build a coupled physical and chemical model of core formation, bringing together cutting edge approaches within experimental geochemistry, computational mineral physics, and fluid dynamic modeling. This effort is directly relevant to Emerging Worlds and NASA because we focus on “Early Evolution of the Solar System” (2.2 Scope of Program for Emerging Worlds) and more specifically on the “period of accretion or the time of global differentiation.” Our efforts with experimental geochemistry will focus on defining the partitioning behavior of key siderophile elements up to the most extreme pressure and temperature (P-T) conditions applicable to core formation. The equilibrium distribution of elements during core formation is dictated by partitioning reactions between metal and silicate, but partitioning reactions remain largely unstudied under the extreme P-T conditions applicable to core formation within larger terrestrial planets. In the absence of directly applicable partitioning data, large extrapolations are currently required predict metal-silicate chemistry in core formation models. We propose to negate the need for P-T extrapolation by measuring the partitioning of key siderophile elements over the entire applicable range of P-T conditions. We will complete partitioning experiments using laser-heated diamond anvil cells and multi-anvil presses. Our focus is on siderophile elements because they are the

most sensitive recorders of the core formation process. Our efforts within computational mineral physics and fluid dynamic modeling are motivated by the fact that equilibrium was not uniformly established between metal and magma during core formation. Rather, as metal descends within magma oceans, it is broken into progressively smaller droplets, but these droplets can remain sufficiently large and spatially concentrated such that little net reaction with silicate occurs during their descent through the magma ocean. A key parameter here is the diffusive length scale of siderophile elements ratioed to the length scale of disrupted metal droplets. This ratio helps determine the potential for chemical exchange. We propose two efforts to quantify the potential for chemical exchange between metal and magma during periods of magma ocean in response to different fluid dynamic scenarios. We will compute, using first-principles molecular dynamics, the transport properties of metal and magma under extreme P-T conditions. This will yield new estimates for fluid viscosity, fluid densities, and diffusivity of key siderophile elements in both magma and metal. We will also complete fluid dynamic modeling to predict the efficiency of metal drop dispersion in response to a variety of initial conditions for magma oceans. Our fluid dynamic modeling is designed to chart flows ranging from the magma ocean-scale dynamics to the breakup of individual metal drops. Our combined efforts will yield the most integrated model of core formation attempted to date.

Noriko Kita / University Of Wisconsin, Madison

Al-Mg Chronology and Isotope Signatures of Chondrules: Unravelling the Diverse Forming Environments in the Protoplanetary Disk

Chondrules in primitive meteorites formed by transient heating in the proto-planetary disk and postdated the oldest refractory inclusions (Ca, Al-rich inclusions; CAIs) by 2-5 million years (Ma). They were likely formed by mechanism that involve growth of planetary system, such as proto-Jupiter, planetary embryos, impacts between planetesimals. Oxygen three-isotope systematics among chondrules have indicated a variety of precursor solids with distinct oxygen isotopes and different environments of their formation. Under the assumption of homogeneous distribution of 26Al (half-life of 0.7 Ma), studies on the Al-Mg chronology of chondrules suggest that chondrule formation ages are systematically different among chondrite groups; chondrules in ordinary chondrites (OC) formation in the inner disk at 1.8-2.2 Ma, which are systematically older than those in carbonaceous chondrites (CC), typically 2.2-2.7 Ma for CO, CM, CV, and Acfer 094 chondrites, and >3-4 Ma after CAIs for CR, CH, CB (CR-clan) chondrites. Systematic investigation of formation ages at higher precisions (0.1-0.2 Ma) are required to fully resolve detail systematics against their chemistry and oxygen isotope signatures. Nucleosynthetic anomalies in 54Cr and 50Ti show two distinct systematic changes between carbonaceous chondrites (CC) and other meteorites (NC), which is known as isotope dichotomy and may help us to understand mixing of solids in the history of protoplanetary disk. However, investigations 54Cr and 50Ti anomaly among individual chondrules, especially those coordinated with oxygen isotopes and Al-Mg chronology are scarce. Task -1: We propose to conduct high time-resolution (<0.1 Ma) Al-Mg chronology of 15-20 chondrules in pristine CV, CM, CO, CR chondrites, which are combined with detailed petrology, oxygen three-isotopes. Least

metamorphosed and aqueously altered carbonaceous chondrites are carefully selected. Silicate Mg# (= [MgO]/ [MgO+FeO] mole%) and mass independent fractionation of oxygen isotope ratios would indicate dust density of local disk and abundance of 16O-poor water ice in chondrule precursor solids. For selected chondrules in CV and CR, we will extract chondrules after SIMS analyses and obtain nucleosynthetic anomalies of 54Cr and 50Ti by using TIMS and ICPMS, respectively. Furthermore, we produce Na-rich plagioclase standards in order to improve accuracy of Al-Mg isochron ages to be better than 0.1 Ma. Task -2: W we examine detail oxygen three isotope systematics of Al-rich chondrules (ARC) in CV and CO chondrites. Some ARCs show internally heterogeneous oxygen isotopes with extreme 16O-rich isotope signatures, close to those in CAIs. Examination of oxygen isotope zoning in each ARC would help understanding the isotope exchange between 16O-rich chondrule melt with surrounding 16O-poor ambient gas. We will determine Al-Mg ages of ARCs to understand possible 26Al heterogeneity and formation time. From the results, we will determine the total range of Al-Mg ages for each chondrite and evaluate any correlation between ages, chemical and isotope variabilities. We address following questions in order to better understand the mechanism of chondrule formation and the evolution of protoplanetary disk: (1) Distribution of chondrule formation ages: Short time intervals (d0.1 Ma) or continuous formation (>0.5 Ma), which may relate to different chondrule formation mechanisms. (2) Younger ages for FeO-rich chondrules than FeO-poor chondrules in CC may imply increase of disk density and decrees of disk temperatures with time. (3) Evidence for radial transport of chondrules, such as older chondrules in CCs show NC-like isotope signatures. The proposed research is to explore the evolution of solids in the protoplanetary disk through the chemical and isotopic properties of extraterrestrial materials that represent primitive solids in the early Solar System. Therefore, it is relevant to the scope of the Emerging Worlds Program.

Francis Nimmo / University Of California, Santa Cruz
Moderately volatile elements as a probe of planetary accretion

Objectives: The patterns of moderately volatile element (MVE) depletion in the silicate portions of planetary bodies arise from two main processes: volatile loss (or incomplete condensation); and core formation. The objective of this proposal is to combine models of planet growth and volatile loss with element partitioning experiments and calculations to explore the origin of the MVE patterns in Earth, Mars, Vesta and the Angrite Parent Body (APB). In particular, we will investigate whether volatile loss from partially-molten planetesimals can explain the observations, and whether conventional or “Grand Tack”-style accretion models work better. Methods: We will begin with our existing core formation model coupled to dynamical accretion simulations. Successful simulations are required to match the non-volatile element concentrations (V,Cr,Co,Mo) and timings from the Hf-W system for Earth, Mars and Vesta. For Earth, nucleosynthetic Mo isotope measurements (indicating contributions from both reservoirs) must also be matched. We will also carry out high-pressure experiments to determine the partitioning of Pb and Ag. Successful core formation models will then be used with existing and our new partitioning data to predict the expected MVE concentrations (e.g. Pb, Ag, Zn, Rb, Ge, K, Cu, Na, Mn, Li, Co, Ni). Discrepancies between the measured and predicted

concentrations will indicate volatile loss or incomplete condensation. Here we will focus on the former as an end-member, based on isotopic evidence of loss of Si and Mg. To model volatile loss, we will begin with the parameterization of Sossi et al. (2019). This shows that volatile loss depends primarily on the melt temperature and the oxygen fugacity. The oxygen fugacity and growth histories of planetesimals are set by the core formation and accretion models; the remaining variable is the temperature distribution. Initially we will treat this as a free parameter and use Monte Carlo simulations to determine what kinds of distributions are acceptable. Preliminary tests suggest a bimodal temperature distribution works well. We will then proceed to investigate the physics of melt production and volatile loss. We will track planetesimal growth and melting from impacts, to determine when and for how long magma is exposed at the surface. We will track the evolution of elemental and isotopic concentrations using the approach of Young et al. (2019). The evolving size of the planetesimal is important to include as volatile loss shuts down for roughly Moon-mass objects, and so too is the mixing of planetesimals having experienced different histories. The model timing of volatile loss is particularly important for the Pd-Ag and U-Pb systems, which are chronometers similar to Hf-W but sensitive to volatile loss as well as core formation. We will track the evolution of these isotopic systems for comparison with available measurements. Significance: This proposal will examine three big questions: whether volatile loss during planetesimal growth is responsible for the elemental depletion patterns; what style of planetary accretion (e.g. Grand Tack vs. conventional) is most consistent with the observations; and when volatile loss happened during the accretion process. Even partial answers to these questions will sharpen our picture of how accretion proceeded in this solar system, and will make predictions (e.g. Ag isotopic signatures for Mars) which are testable. Relevance: This project examines processes operating during the accretion of planetesimal- and embryo-size objects. It is therefore relevant to the EW objectives, and specifically fits within "studies related to the accretion of Solar System bodies after dissipation of the protoplanetary disk".

Karin Oberg / President and Fellows of Harvard College
Decoding the Isotopic Fingerprints of Solar System Volatiles: A Laboratory Investigation of Isotopic Fractionation Chemistry in Interstellar Ice Analogs

Context: Molecular isotopic ratios are frequently used to assess the origins of volatiles in Solar System bodies. A notable example is the use of the D/H ratio of the Earth's water to constrain its origin. Generally, excess D/H ratios in water and volatile organics are thought to originate from cold chemistry in interstellar clouds. The D/H ratios found in Solar System bodies also depend, however, on isotopic alterations that occurred between volatile formation in the pre-Solar cloud, and incorporation into Solar System bodies. Our ability to interpret Solar System D/H ratios is currently limited by a lack of data on possible alteration processes. Our understanding is especially limited for solid-state processes, i.e. on deuterium exchanges in Solar Nebula ices, scrambling the original deuterium record, and on deuterium loss due to ice chemistry. Objectives: The objectives of our study are to experimentally characterize and quantify water and organic ice deuterium depletion, and water-organics deuterium exchange mechanisms. In the Solar Nebula icy grain mantles would have been exposed to atom bombardment, UV radiation,

electrons, and heat, all of which could affect the isotopic composition of both the water ice matrix, and of embedded organic molecules. We will explore how different kinds of ice processing affect the isotopic composition of pure and mixed ices. Methods: To achieve our objectives we will run a series of ice experiments in a dedicated ultra-high vacuum set-up. In each experiment we will first deposit a thin pure ice, or water:X ice mixture, where X is methane, methanol, ammonia or hydrogen cyanide. The ice (mixture) will be monitored using infrared spectroscopy complemented by mass spectrometry while the ice is being heated, and/or exposed to H or D atoms, UV photons or electrons. The resulting spectroscopic time series will then be used to derive deuterium depletion and exchange rates in each experiment. The results will be used to construct simple models of water and organic ice deuterium depletion and exchange chemistry under different nebular conditions. Relevance: The Emerging Worlds program, as stated in the 2020 ROSES call, aims to answer "the fundamental science question of how the Solar System formed and evolved", including studies of all aspects of materials and processes occurring in and affecting protoplanetary disks, such as the Solar Nebula. Our goal is the development of a holistic view of the origin of observed deuterium fractionation levels in water ice and organic ices in the Solar System, and further to unlock the full potential of D/H measurements of Solar System volatiles to trace the histories of these volatiles, and of their parent bodies. Increasing our ability to decode the isotopic fractionation patterns of Solar System volatiles would directly support a range of previous, existing, and future NASA funded research and missions aimed at measuring the isotopic compositions of Solar System volatiles.

Maxime Ruaud / SETI Institute
Tracking Reservoirs of Deuterium in the Early Protosolar Disk

Chondrites and comets are believed to be the sources of water, volatiles (including noble gases), and organics to the terrestrial region during early epochs of solar system formation. The D/H ratio of water and organics in these bodies varies significantly, with chondritic water values being intermediate to the solar and Earth values and comets having a D/H ratio in water that ranges from terrestrial to the high ratios found in interstellar cloud material (Alexander et al. 2018, Space Sci. Rev., 214, 36). D-enrichment and depletion ratios have been used to infer the origin of Earth's water and to infer the range of radial distances where comets may have formed. The D/H ratio is a unique indicator of the radial compositional gradient in the presolar disk; determining this signature could provide valuable insights to the formation location of meteorite parent bodies and comets and indirectly infer the dynamical history of the early solar system. Current investigations attribute much of the observed D/H enrichment as being inherited from the presolar cloud material. This is supported by the similarity in the range of D/H ratios determined from studies in the interstellar medium and from theoretical work that follow the evolution of the composition of ices from the prestellar core stage to the formation of Class I circumstellar disks (e.g. Furuya et al. 2017, A&A, 599, 840). In particular, the predicted ratio of [D2O/HDO]/[HDO/H2O] from these models can successfully explain that found in comet 67P (Altwegg et al. 2019, ARAA, 57, 113). However, although Furuya's model indicates cometary water to be of interstellar origin, comets and meteorites parent bodies are likely to have formed at a later Class II stage

(>1-3 Myr) of the protosolar disk and the D/H ratio is unlikely to have been preserved because of the effects of transport and dust evolution. In fact, the physical conditions in the protosolar disk, for example the mass, temperature and gas/solids ratio, must have widely differed both in space and time as it evolved to form planets, comets and asteroids. As dust particles migrate, collide, fragment and/or settle toward the disk midplane with time, the average dust cross-sectional area varies radially and vertically throughout the disk, affecting the penetration of FUV photons as well as its density and temperature structure. As a result, an evolving dust grain population could have had a major influence on protosolar disk chemistry and thus an impact on the deuterium fractionation of both water and organics found in comets and meteorites. Here we propose to investigate deuteration in the solar nebula using state-of-the-art chemical models and consider disk evolution and transport processes. In recent work, we coupled a full thermo-chemical disk model with a gas-grain chemical model to calculate the chemistry in disks with updated 2D treatment of the photoprocesses (Ruaud et al. 2019, ApJ, 885,146). One of our main conclusions is that the photoprocesses dominate chemistry; not only in the outer disk and in the disk atmosphere, but also on ices close to the disk midplane. For this project, we will consider the formation of deuterated species on ices beginning from the presolar cloud core (interstellar material) and follow their evolution through the disk on simple molecules and on more complex organic species which may be the precursors to the IOM material seen in meteoritic bodies. We will use available gas-phase deuterated networks (Majumdar et al. 2017, MNRAS, 466, 4) and build the grain surface network from published data found in the literature. We will thus infer the effect of updated photoprocesses on D/H ratios and determine the inventory of deuterated complex organic molecules in disks. Results from this project will compared to measurements from Solar System's primitive bodies.

Sarah Stewart-Mukhopadhyay / University Of California, Davis
The Thermodynamics of Building Earth-like Planets

This work seeks to investigate the thermodynamic properties of rocky planets during collisional growth, which are necessary to understand how elements are distributed between mantles and cores during differentiation and to be able to study the incorporation of volatiles into the final planets. We propose to (1) measure experimentally key thermodynamic parameters of major planetary minerals and rocks using multiple dynamic compression techniques; (2) incorporate these new data with existing and ongoing data obtained by static techniques and ab initio calculations to develop new equation of state models for terrestrial mantles and crusts; (3) to conduct numerical simulations of planetary collisions to address key questions related to the pressure-temperature conditions for core formation, the thermodynamics of escaping ejecta, and collisional processing and erosion of early crusts; and (4) to publish and curate well-documented open-access equation of state models for wide use in studies of planetary interiors and dynamic processes. The proposed experimental work will be conducted in the PIs Shock Compression Laboratory at UC Davis. This facility contains two light-gas guns that can generate shock pressures up to Earths core conditions. These data will be combined with shock data obtained separately on laser and pulsed power platforms by the PIs group. By combining several types of shock thermodynamics experiments on

different platforms, we obtain shock Hugoniot states and constraints on the heat capacities and Gruneisen parameters of planetary materials. In addition, ab initio calculations by Collaborator Razvan Caracas will supplement these data under conditions that cannot be explored experimentally. Here, we will focus on developing equation of state models for a mantle (pyrolitic) composition and crustal (basaltic) composition appropriate for the period of planet growth. The PIs group has previously improved the development of wide-ranging equations of state models using the ANEOS code package. In this work, we will extend these models to include multiple solid phases. These data products will be publicly released and have a wide-range of applications in planetary studies of rocky planets up to Super-Earth masses. The specific applications of our numerical models, using our updated equations of state, will focus on understanding the pressure-temperature distributions in rocky planets during accretion. Previous work has found that the energy and angular momentum from giant impacts leads to much lower interior pressures and higher temperatures than currently considered in studies of core formation. Our preliminary work demonstrates that portions of the mantles and cores become supercritical fluids during giant impacts. This work will provide essential information to be able to understand the chemistry of Earths accretion and will help resolve several outstanding questions about the geochemical properties of rocky planets. By providing more accurate temperatures, our work will inform studies of the partitioning of elements into the core and mantle. This work supports the Emerging Worlds program by investigating a major physical process during planet accretion.

Kathryn Volk / University Of Arizona

Constraining Neptunes migration using the surface properties of resonant trans-Neptunian objects

Overview: The trans-Neptunian region's complex dynamical structure was largely sculpted by giant planet migration. However, details of this migration are still uncertain: How far did Neptune migrate? Was it smooth or 'grainy'? Were there significant jumps? Cold classical TNOs (objects on low-eccentricity, low-inclination orbits from 42-48 au) are thought to have formed in situ. Neptune's 2:1 mean motion resonance lies just exterior to this population. During Neptune's migration, the 2:1 had to either pass through or possibly skip over the cold classical TNOs. Recent observations reveal that the cold classical TNOs' surface properties are distinct from those of the dynamically excited TNOs (thought to originate inside 30 au). Objectives: We will measure the distribution of surface properties in Neptune's 2:1 resonance (Task 1), providing a novel observational constraint on the number of cold classical TNOs captured during migration. We will model the final stages of Neptunes migration to predict the population of captured cold classicals in the 2:1 as a function of the currently unconstrained migration parameters (Task 2). We will then directly these models against the observations (Task 3), providing strong, unambiguous constraints on Neptune's migration. Methods: We will combine analysis of existing observational data, modeling of observational biases, and modeling of Neptune's migration in the early solar system to achieve our objectives. We have already obtained raw observational data of 26 TNOs in the 2:1 resonance using the Large Binocular Telescope (LBT) in the filters that will reveal if any show distinctive cold classical surfaces once the photometry of these TNOs is measured. Observational biases

strongly affect the observed orbit and color distribution of TNOs. Our targets are from the well-characterized Outer Solar System Origins Survey Ensemble (OSSOS+). We will use the OSSOS+ survey simulator to model the biases and determine the intrinsic distribution of surface types for the 2:1 resonance from our observations; this will constrain how much of the 2:1 TNO population was captured from the cold classical region during migration. We perform numerical simulations of Neptune's migration for a variety of migration scenarios, simulating the capture of cold classical TNOs into the 2:1 and other populations. These models will be tested against the observations. Significance: The proximity of Neptune's 2:1 resonance to the cold classical TNOs provides a unique opportunity to use TNO surface properties to trace Neptune's migration. The well-constrained current-day cold classical population can be treated as an absolute lower limit on the number of cold classicals the 2:1 had to traverse as Neptune migrated. If the cold classical population was more numerous or dynamically colder before migration (both likely), capture by the 2:1 would only increase. We can thus place robust lower limits on the number of captured cold classical objects in the 2:1 today for different planetary migration scenarios, and we expect to falsify many of the possible migration scenarios. By combining dynamical models with our observational results, we will place new and very strong constraints on Neptune's migration history. Relevance: Our proposed investigation of the early solar system focuses on constraining planet migration, which happened "between the time of Solar System formation and the time that large planetary bodies were in or near their modern configuration", and thus falls into the scope of Emerging Worlds. While our project does contain an observational component, it is anticipated to be limited to analysis of existing data, and the primary science focus is the modeling to interpret that data. This project thus falls outside the scope of Solar System Observations, which "must contain as a primary focus new observation of Solar System objects (excluding Earth and Sun) during the proposed period of performance."

Richard Walker / University of Maryland, College Park
Characterizing Hafnium/Tungsten Ratios in Bulk Chondrites

The proposed research is to improve our understanding of the possible variance in hafnium/tungsten (Hf/W) ratios among bulk chondrites. The elements Hf and W comprise the short-lived 182Hf-182W system (t_ = 9 Ma), which is now widely used to place constraints on the timing of metal-silicate differentiation of planetary bodies via the analysis of iron meteorites, as well as thermochronology of primitive meteorites. The Hf/W ratio of bulk planetary bodies is important because it determines the tungsten isotopic evolutionary path prior to primary differentiation into core and mantle. Thus, it is a critical variable in calculating 182W model metal-silicate segregation ages of iron meteorites, and metal phases separated from other types of meteorites. At present, however, such age calculations are typically calculated assuming an average Hf/W ratio determined for carbonaceous chondrites. Based on the isotopic systematics of ordinary chondrite components, however, some recent studies have concluded that the Hf/W of the parent bodies of ordinary (and possibly enstatite) chondrites were significantly lower than for carbonaceous chondrites. This conclusion is supported by a very limited number of

analyses of bulk chondrites. If correct, this means that some reported segregation ages for noncarbonaceous type (NC) irons may be too old. This is an important issue as, for example, the veracity of such ages weighs heavily in attempts to account for the causes of genetic differences between NC and carbonaceous (CC) reservoirs. In addition to its chronological applications, accurately constraining the ratio of a lithophile (Hf) to a moderately siderophile (W) element in bulk primitive meteorites may provide fresh insights to metal-silicate sorting or other early processes in the nebula. The primary goal of this proposal is to measure Hf/W, 182W/184W and 183W/184W ratios in bulk samples of ordinary, enstatite and carbonaceous chondrites, applying current state-of-the-art, high-precision measurement methods. The study will utilize a two-pronged approach: a) measuring relatively small masses (~1 g) of ~25 bulk chondrites in order to update the number and precision of data available for chondrites, and b) measuring comparatively large masses (~5-10 g) of a total of ~5 bulk ordinary and enstatite chondrites, in order to assess the effects of metal-silicate heterogeneity on Hf/W ratios in chondrites containing a substantial metal component. Methodology: We have previously developed chemical separation techniques to separate Hf and W from chondritic materials for concentration and isotopic compositions. Hafnium and W elemental abundances will be measured by isotope dilution using multi-collector inductively-coupled plasma mass spectrometry, and W isotopic compositions will be made using either thermal ionization mass spectrometry or multi-collector inductively-coupled plasma mass spectrometry. All necessary instrumentation is available at UMd. Relevance: All of the proposed work is directed towards the stated goals of the Emerging Worlds program which "aims to answer the fundamental science question of how the Solar System formed and evolved" (page C.2-1, ROSES 2020). In this case the research will have a direct impact on how Hf-W model ages are calculated.

Richard Walker / University of Maryland, College Park
Characterizing the Genetics of Lunar Basin-Forming Impactors Using Ruthenium Isotopes

Goals, Significance, and Perceived Impact. We propose to apply Ru isotope analytical methodology to investigate the genetics of the basin-forming lunar impactors that dominate the HSE present in lunar impact melt rocks. Evidence from meteorites and early-Earth rocks provides evidence for large-scale Ru isotopic heterogeneity within the protosolar accretionary disk. This means that Ru isotopes can be used as a powerful genetic tracer to distinguish among some possible meteorite classes that have previously been proposed for basin-forming impacts on the Moon, e.g., enstatite vs. carbonaceous chondrites. All rocks planned for analysis have been previously well-characterized for HSE abundances and Os isotopic compositions. Among other objectives, this work should reveal whether or not CC-type impactors were significantly involved in the basin-forming events on the Moon. The CC-type meteorites have generally been assumed to have formed outboard of the proto-Jupiter, and so identification of a major CC component in impact melt rocks could lead to an interpretation of a specific category of dynamical delivery. The results may also provide additional evidence for the s-process enriched component observed in rocks from SW Greenland. During the 2 year period of funding requested, we propose to make Ru (and bulk HSE and Os isotopic)

measurements of ~30 Apollo samples, using a state-of-the-art, multi-collector inductively coupled plasma mass spectrometer. Results should allow us to discriminate between impactors dominated by NC vs. CC components. Ultimately, the results of this study may allow an assessment of whether or not some basin forming impactors were derived from the inner or outer solar system, and by inference, whether the basin forming impactors possibly provided substantial water and/or organic matter to the inner solar system. Methodology: The methods for achieving the analytically challenging goals of this proposal are mostly in place at the UMd. We have previously developed methods for cleanly and efficiently separating Ru from various types of matrices. Silicate-rich samples, such as impact melt rocks, are digested using a combination of nitric and hydrochloric acids in sealed Pyrex Carius tubes at 260°C. Ruthenium is initially purified from other elements using anion exchange chromatography, followed by a final stage purification achieved by micro distillation. We have been developing methods to precisely measure the 100Ru/101Ru of ~35 ng of Ru to a precision of ~+/-12 ppm, using our Thermo-Fisher Neptune Plus multi-collector inductively coupled plasma mass spectrometer. We anticipate a ~2 month developmental period to achieve this objective. Relevance: All of the proposed work is directed towards the stated goals of the Emerging Worlds program which "aims to answer the fundamental science question of how the Solar System formed and evolved" (page C.2-1, ROSES 2020). In this case the research will address the origin of later stage impactors, possibly representing what some have termed "late heavy bombardment", to the inner Solar System.

Kun Wang / Washington University
Experimental Studies of Volatile Fractionation in the Early Solar System

SCIENCE GOALS AND OBJECTIVES: The differentiated planetary bodies of the solar system such as the Earth, Moon, Mars, and asteroid 4 Vesta are depleted in moderately volatile elements (e.g., Na, Cl, K, Cu, Zn, and Rb) in various degrees compared with undifferentiated meteorites such as carbonaceous and ordinary chondrites. The reason of such moderately volatile element depletion in planetary materials is still under debate. Possible mechanisms include 1) incomplete condensation in the solar nebula; 2) partial evaporation during planetary accretion; 3) magma ocean degassing; and 4) local volcanic outgassing. Coupled isotopic studies using Zn, K, and Cu isotopes in a range of volatility (50% condensation temperatures from 726K, 1006K, to 1037K) can potentially distinguish these different mechanisms. However, there are no coordinated laboratory experiments yet to provide any constraints on equilibrium/kinetic isotopic fractionation factors during vaporization and condensation as a function of P, T, fO2 and starting compositions. Specifically, we are going to propose two tasks here: 1) to calibrate equilibrium K isotopic fractionation factors between melt and vapor at temperatures between 1200 to 2000 °C through Knudsen effusion cell experiments; 2) to study coordinated kinetic elemental and isotopic fractionation of Zn, K, and Cu in open systems by vaporizing natural and synthetic samples under controlled oxygen fugacities in gas mixing furnaces at pressures between 10-4 to 1 bar. The results of these experiments under kinetic and equilibrium conditions would be used to compare to the measurements of Zn, K, and Cu isotopes in chondrites and samples from the Earth, Moon, Mars, and

Vesta to understand what are the processes and what are the conditions that are responsible for the moderate volatile element depletions in the Early Solar System. METHODOLOGY: Two types of experiments will be conducted. First, at equilibrium conditions, we will use custom-made Knudsen effusion cell facility at Missouri State University to achieve melt-vapor equilibrium at temperatures between 1200 and 2000°C and the quenched melts will be recovered for the elemental and isotopic study. Second, at kinetic conditions, we will perform open-system vaporization experiments on natural samples at temperatures between 1200 and 1650°C and at pressures between 10-4 to 1 bar using Deltech controlled atmosphere vertical tube furnace systems at Washington University in St. Louis. All experiment products (evaporation residues) will be first examined with EMPA (electron microprobe analysis), and their bulk major and trace elements will be measured with Thermo Scientific iCAP Quadrupole ICP-MS (Inductively-Coupled-Plasma Mass-Spectrometer) at Washington University in St. Louis. The Zn, K, and Cu isotope compositions of these evaporation residues will also be analyzed with Neptune MC-ICP-MS (Multiple-Collector Inductively-Coupled-Plasma Mass-Spectrometer) at Washington University in St. Louis. RELEVANCE: This study is highly relevant to NASA's scientific goals. It addresses the strategic science question of NASA planetary program that "explores and observes the objects in the Solar System to understand how they formed and evolve" by understanding what early thermal and/or chemical processes have (in various degrees) deprived of volatiles from terrestrial planets (e.g., Mars and Moon) and minor bodies (e.g., asteroid 4 Vesta and Angrite Parent Body) in the early history of the solar system. The results produced by this study will facilitate the interpretation of orbital and ground observations from the current NASA missions to Mars, 4 Vesta and other asteroid belt objects, and assist the planning of future missions to the Moon and other inner solar system objects. This proposal directly answers the calls described in Section 2.2 of C.2 "Early evolution of the Solar System."