What is Mineral Informatics?

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Abstract: Minerals are information-rich materials that offer researchers a glimpse into the evolution of planetary bodies. Thus, it is important to extract, analyze, and interpret this abundance of information in order to improve our understanding of the planetary bodies in our

solar system and the role our planet's geosphere played in the origin and evolution of life. Over the past decades, data-driven efforts in mineralogy have seen a gradual increase. The development and application of data science and analytics methods to mineralogy, while extremely promising, has also been somewhat ad-hoc in nature. In order to systematize and synthesize the direction of these efforts, we introduce the concept of "Mineral Informatics". Mineral Informatics is the next frontier for researchers working with mineral data. In this paper, we present our vision for Mineral Informatics, the X-Informatics underpinnings that led to its conception, the needs, challenges, opportunities, and future directions. The intention of this paper is not to create a new specific field or a sub-field as a separate silo, but to document the needs of researchers studying minerals in various contexts and fields of study, to demonstrate how the systemization and increased access to mineralogical data will increase cross- and interdisciplinary studies, and how data science and informatics methods are a key next step in integrative mineralogical studies.

Keywords: Minerals; X-Informatics; Data; Data Science; Information; Scientific Discovery.

Word Count: 15714

1. Introduction

The potential for data-driven methods to make novel, unintuitive, and groundbreaking discoveries in Earth and planetary science research will only grow as the volume and

variety of data increases with time. Mineralogy, in particular, is ripe for the application of data-driven methods. Minerals form as a result of their unique chemical and physical conditions and, in the process, retain information regarding their formation information that offers an opportunity to study the complex geologic and biologic past of these planetary bodies (Prabhu et al. 2021a).

Mineralogy has been the subject of scientific curiosity and study for millennia (Needham 1986; Bandy & Bandy 1955). In addition to their roles as captivating specimens for collection and study, minerals and their ores are essential in the survival and industrialization of humankind (Murray 1995; Coates 1985). This interest and utility has led to the characterization and systemization of mineralogy and mineral occurrence on Earth and other planetary bodies (Dana & Dana 1895; Hazen & Morrison 2021; Bragg and Bragg 1913; Strunz & Tennyson 1941; Lafuente et al. 2015; Lehnert et al. 2000). As a result of this rich history of scientific investigation, vast amounts of information are available on the occurrence and attributes of minerals. These data provide a robust platform for the analysis of more complex, multidimensional, and larger mineralogical systems; the integration of heterogeneous data types, linking to data from other fields of science; and predictive, data-driven scientific exploration - all of which leads to the answering of complex, multidisciplinary questions. The potential of data-driven mineralogical research has been exemplified by important scientific advances in the last decade. Recent discoveries have demonstrated periodicity of mineral formation and diversification associated with supercontinent assemble (Bradley 2011; Voice et al. 2011; Nance et al.

2014; Hazen et al. 2014), an association of mineral redox state to the oxidation of Earth's atmosphere (Liu et al. 2021; Hummer et al. 2022; Large et al. 2022), and that much of Earth's mineral inventory is the direct or indirect result of interactions with water and/or biology (Hazen & Morrison 2021, 2022), as well as the prediction of the number of as-yet undiscovered mineral species (e.g., Hazen et al. 2015, Hystad et al. 2019; Hystad et al. 2015), the chemical composition of minerals on Mars (Morrison et al. 2018 a-c), and the location of undiscovered mineral deposits (Prabhu et al. 2019; Morrison et al 2022 (in prep)). Mineralogy is rapidly entering the data-driven era, tackling previously unanswerable questions, and demonstrates the need and opportunity for a symbiotic relationship between the mineralogy and the fields of data science and informatics.

Data-driven efforts in mineralogy have been gradually increasing in the past decades and there are some promising studies that have helped researchers uncover the patterns hidden in the data and have led to scientific discoveries (Morrison et al 2017; Hazen et al. 2019; Prabhu et al. 2019; Morrison et al 2020; Hazen & Morrison 2020, 2022; Zhao et al. 2020; Gregory et al. 2019; Boujibar et al. 2021; Hystad et al. 2021). While still nascent, application of data science and data analytics methods in mineralogy shows a promising trajectory. The development of these methods and advances in the past have been somewhat ad-hoc in nature. However, development of mineral informatics can be guided in a more deliberate and systematic way by taking into account the underpinnings from information theory and data science advances, as exemplified by collaborations in other fields, including biology, medicine, chemistry, and astronomy. We believe this is the start

of a new era in mineralogy, where utilizing data-driven methods to answer mineralogical (and broader scientific) questions takes center stage.

In this paper, we take a high-level look at our vision for "Mineral Informatics", the underpinnings that led to its conception, the needs, challenges and opportunities for this emerging field of mineral informatics. We also discuss the implications such advances will have on the field of mineralogy.

2. Foundation provided by X-informatics

Informatics studies the structure, algorithms, behavior, and interactions of natural and artificial systems that store, process, access and communicate information (Fox 2011). The term informatics has often been used in conjunction with the name of a domain/discipline, for example, Bioinformatics, Geoinformatics, Astroinformatics, and Cheminformatics. In the past, researchers with expertise in a specific domain worked on processing and engineering information systems designed for that domain only. But in the last decade, informatics has gained a much wider visibility across a range of disciplines (Prabhu 2018). This wider visibility is in large part due to successful efforts at systematizing the core (i.e., discipline neutral) aspects of informatics, for example, use-cases, human-centered design, iterative approaches, information models etc. (Fox 2020). The core methods of informatics are used as a foundation to explore raw data and extract

information from the data that lead to scientific discoveries. As the volume and complexity of the data increase, so does the need for utilizing the solid foundations provided by informatics methods and combining them with needs of the specific domain to pursue data-driven scientific discoveries.

Mineral informatics is a nascent approach compared to fields like Bioinformatics, Medical Informatics, and Geoinformatics that have been pursued for decades (Collen 1986; Sinha 2006; Fox et al. 2006; Gauthier 2019). The intention of this paper is not to create a new specific field or a sub-field as a separate silo, but to think of and document the needs of researchers studying minerals in various contexts and how data science and informatics methods are a key next step in mineralogical studies. We also need to learn from the successes and failures of more mature domains that have applied the informatics approach. Lastly, a very important factor to keep in mind is the truly interdisciplinary and important questions that can be explored by studying minerals. So, while the term "mineral informatics" may seem like creating a new subclass of geoinformatics, we assert that we are instead tying in various disciplines that use minerals as a key part of the pursuit for answers to big science questions.

3. A methodology for mineral informatics explorations

In this paper, we present a general methodology for mineral informatics (see Figure 1). This methodology, adapted from Fox & McGuinness (2008), includes all the steps typically

followed in a data-driven scientific exploration. This approach was created for mineral informatics but, as is the case with many data science and informatics approaches, is transferable and applicable to other domains.

Most informatics explorations start in one of two ways: 1) Scientists have a research question they want to answer, or 2) scientists have data ready to be explored. In the second case, we perform preliminary data exploration, which helps generate new hypotheses and research questions based on interesting trends and anomalies in the data.

Once a specific research question has been selected for scientific exploration, we start by dividing the large problem into smaller more tractable parts. Next, we iteratively develop use cases for every one of these parts. A "use case" is a documented collection of possible sequences of actions and interactions between a system and its users in pursuit of a particular goal. Identification and development of use cases helps to define the needs (e.g., data, personnel, infrastructure) for this data-driven approach. The next steps in the methodology includes creating (or assigning roles to an already established) an interdisciplinary team to conduct the data-driven research.

Next, we inventory the preliminary dataset and/or existing mineral data resources (See section 5a) to determine if they are what is necessary for the desired exploration. In some cases, we need to collect, compile, and extract data from other repositories or sources like scientific literature, websites, digital PDFs, and experimental results. We then create

an information model to better understand and mediate data from heterogeneous sources and data types, which provides a holistic picture of the relationships between the various data sources, types, and attributes. The information model allows us to extract the datasets and data attributes most relevant to answering the desired research question. Note that this step differs from the statistical and machine learning approaches used for feature selection.

We then begin applying data analytics methods (i.e., data visualization as well as descriptive, predictive, and prescriptive analysis) to identify and explore patterns and anomalies seen in the data. A team of domain and data scientists iteratively examine the results of the analytics methods and use their respective expertise to (1) provide interpretations and/or insight, and/or (2) recommend changes to the analysis. The data analysis and scientific interpretation are usually done over multiple iterations with small modifications to the approach, algorithms, and/or code to explore different aspects of the data.

If scientists come to an agreement that parts of the analysis would be widely used in the larger community, they can choose to generalize and adapt their work into a system, technology, or infrastructure. This development can include creation of tools, code snippets, reusable workflows, R packages, Python libraries, and other resources. Irrespective of whether there is a decision to create a general tool, technology, or

175 package, we recommended using rapid prototyping coding practices[1] (Gordon & Bieman
176 1995) for data science and informatics activities.
177
178 After obtaining the desired results from our data analysis, it is important to disseminate
179 and effectively communicate the research products generated by mineral informatics
180 explorations. Research products can include datasets, code, scientific literature,
181 executable workflows, etc. Establishing best practices for disseminating research
182 products is an ongoing effort, especially in the geoscience community. Datasets can be
183 published as part of a data paper, or be assigned their own DOIs by data repositories like
184 Zenodo, Dryad, Figshare, or Dataverse (Assante et al. 2016). Existing mineral data
185 repositories like the EarthChem Library (ECL), Astromat, and the Open Data Repository
186 (ODR) (See section 5a) also provide DOIs for datasets deposited by researchers.
187 Additionally, some journals host data associated with their publications. Similar to
188 releasing data used in scientific exploration, code can be maintained and released in many
189 ways, including Github (with a persistent identifier pointing to the repository), figshare,
190 or Zenodo. Saving executable code for an experiment in an interactive environment like
191 Jupyter or R notebooks adds to the reproducibility of the code and of the scientific
192 workflow in general (Prabhu & Fox 2021). Dissemination of scientific advances through
193 scientific publications has been practiced for more than 300 years (Fyfe et al. 2015). In
194 addition to journal publications, conference proceedings, preprint servers (such as arXiv,

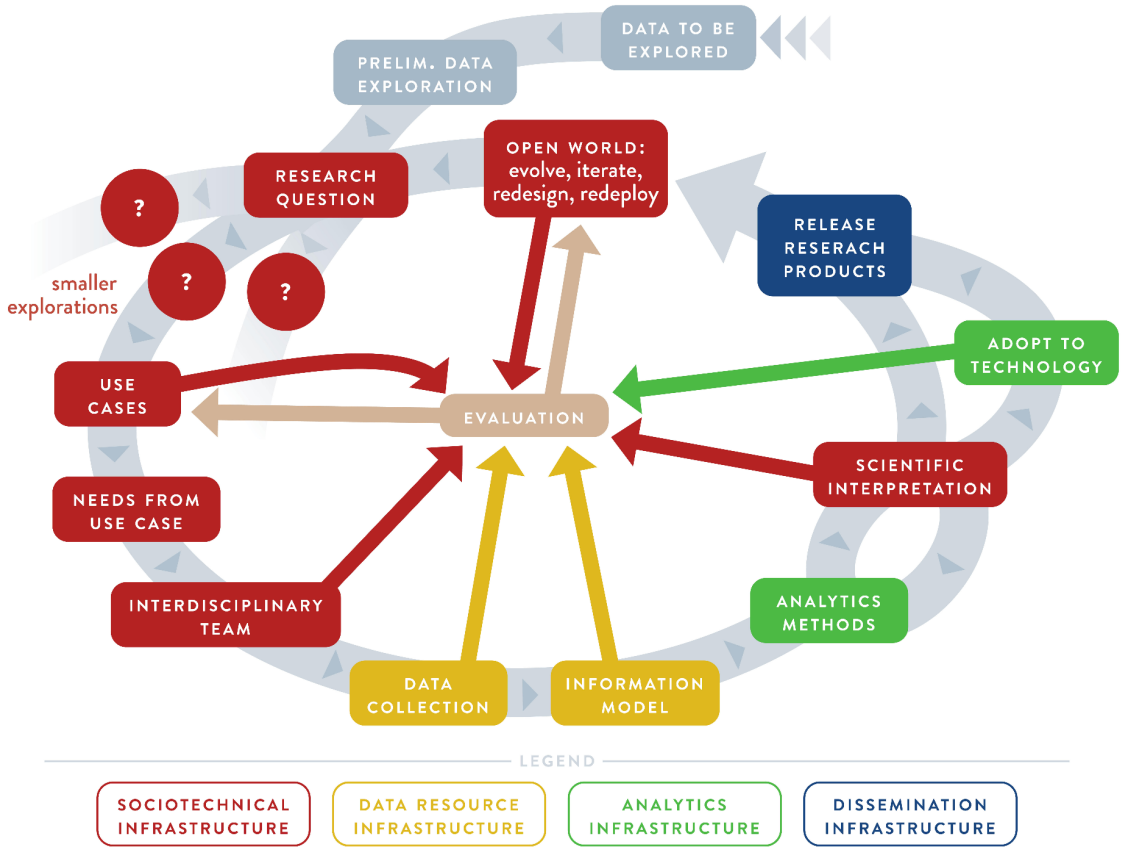
[1] https://medium.com/convergeml/rapid-prototyping-in-machine-learning-ffe79f023aec

ESSOAr, and EarthArXiv), and even press releases associated with publications have considerably improved the landscape of disseminating research products.

The final stage of our informatics methodology follows the sharing of the research products. If researchers follow FAIR and Open Science practices (Wilkinson et al. 2016; Stall et al. 2019; Ramachandran et al. 2020) not only for the dissemination of their scientific results, but also during the use case development, information modeling, and analysis stages, then it becomes easier to evolve, improve, redesign, or adapt your work. Ongoing research and recommendations on designing FAIR and Open scientific workflows will help improve the methodology of data-driven exploration (e.g., Prabhu & Fox 2021; Kluyver et al 2016; Sandve et al. 2013).

It is important to evaluate the outcomes at almost every stage of the informatics methodology. The evaluation method or metric used at each stage will be significantly different, but it is important to stop at the end of every stage and assess not only the progress made, but also lessons learnt for future iterations in the same exploration or the beginning of a different exploration. For example, a data collection/resource may be evaluated based on a set of quality criteria (e.g., Prabhu et al. 2021a), but results from the data analysis may need to use quantitative metrics to evaluate results from a descriptive, prescriptive, or predictive model (e.g., Statnikov et al. 2008; Tomasev & Radovanovic 2016; Hossin & Sulaiman 2015; Zhou et al. 2021). Established evaluation methods exist for each stage of the informatics methodology, and we recommend following those

established best practices and standards set by the scientific community. Issues found during evaluation will need to be documented in the use case and thus improve the data-driven exploration during the next iteration or redesign of the approach.



[Figure 1: Mineral Informatics Methodology]

Caption: Mineral informatics methodology adapted from Semantic Web methodology by Fox & McGuinness (2008).

4. Challenges and opportunities in Mineral Informatics

Mineral informatics methods not only systematize the mineral data landscape, but also provide a path to answering some of the big, interdisciplinary scientific questions. Figure 2 gives an example of the domains influenced by the research questions being broached with mineral informatics methods.

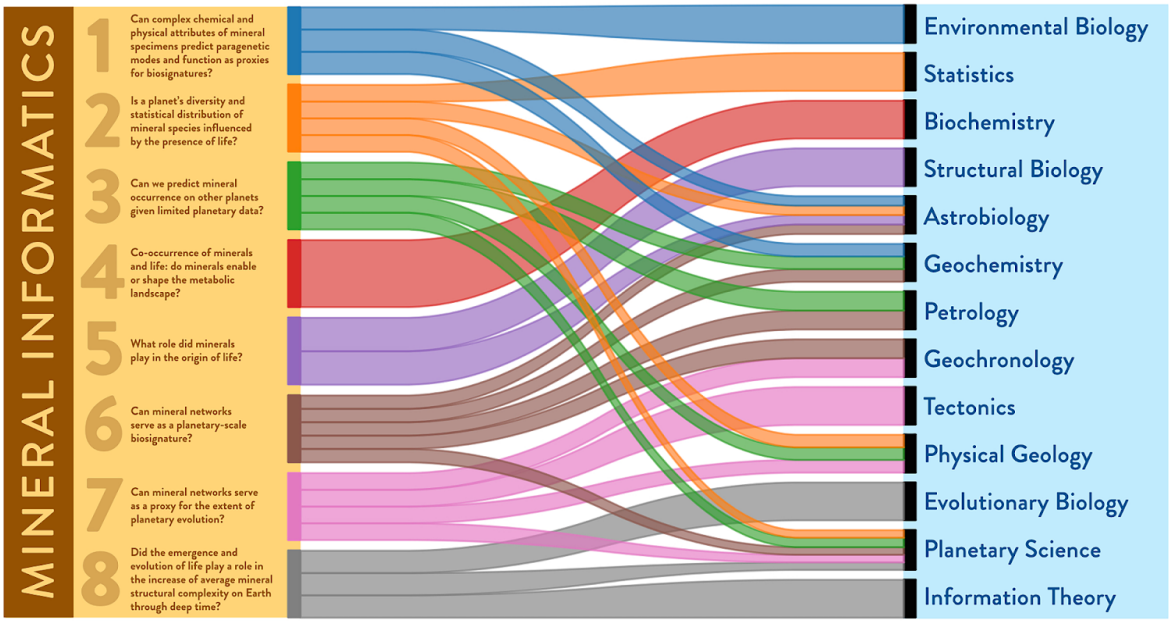


Figure 2: Interdisciplinary research questions related where mineral informatics play a key role.

a. Major scientific questions that can be addressed with mineral informatics

i. Can complex chemical and physical attributes of mineral specimens predict paragenetic modes and function as proxies for biosignatures?

Minerals record the physical, chemical, and, in some cases, biological conditions of their paragenetic modes (i.e., formational and alteration environments). This information is stored in the myriad attributes of mineral specimens, including major, minor, and trace elements, isotopic ratios, texture, and grain size. Therefore, conditions of mineralization, including whether or not there was biological input, can be characterized with cluster analysis performed on the various properties of mineral samples (Gregory et al. 2019). Furthermore, robust classification schemes can be developed from the clustering models that will enable prediction not only of the geologic environment of formation but also of any biogenic origins (Hazen 2019). Therefore, this work will deconvolve our understanding of the minerals that formed in environments influenced by life from those that formed under strictly abiotic conditions.

ii. Is a planet's diversity and statistical distribution of mineral species influenced by the presence of life?

Life creates unique niches of chemical disequilibrium for minerals to exploit. These processes likely drove a significant fraction of the mineral diversity we see on Earth today, influencing the spatial and temporal patterns of mineral distribution (Hazen et al. 2018; Morrison et al. 2020; Hazen & Morrison 2022). These trends on Earth and other planetary bodies can be modeled, compared, and used to develop statistical biosignatures

and abiosignatures regularizing the diversity and distribution of mineral species across a planetary body (Hystad et al. 2019) and provide models for planetary-scale mineralogical biosignatures of inhabited worlds.

iii. Can we predict mineral occurrence on other planets given limited planetary data?

From orbital infrared spectroscopy, we have obtained global or near-global datasets of the mineralogy of other terrestrial worlds, including Mars, Mercury, Vesta, and Ceres (Murchie et al. 2009; de Sanctis et al. 2012; Ehlmann & Ewards 2014; Namur & Charlier 2017; Prettyman et al. 2019). Informatics methods, such as association analysis, can be used to predict the existence of minerals that cannot be detected from space. By understanding mineral affinities for assemblages, localities, and geochemical parameters, we may be able to use a sparse mineralogical dataset to anticipate future discoveries (Prabhu et al. 2019), but first a robust small/sparse-data framework must be developed (see Section 6a). Enhancing predictive capabilities will help to prioritize landing sites for future landers and rovers with broad science goals that relate to mineralogy, like understanding planetary history or searching for signs of life. Such predictions would be strategically important because interplanetary missions cost hundreds of millions to billions of dollars and take years to decades to develop, build, and launch.

We also have geochemical indicators of the mineralogy of the ice-covered ocean world Enceladus from plume flybys and E-ring analyses performed by the Cassini spacecraft (Postberg et al. 2008; Waite et al. 2017; Glein & Waite 2020). Mineral informatics methods can help predict the mineral composition of ice-covered ocean worlds, whose mineralogy is planetologically and perhaps astrobiologically relevant but cannot be accessed directly in the near future.

iv. Co-occurrence of minerals and life: do minerals enable or shape the metabolic landscape?

Minerals play a key role in biological redox transformations. Microorganisms, (e.g., of the genus *Geobacter*) are able to use metals in their environment to power their metabolisms (Childers et al. 2002). Several studies have suggested deep similarities between minerals and metalloenzymes (Nitschke et al. 2013; Zhao et al. 2020; McGuinness et al. 2022 (In Review)). Thus, minerals may play an important role in shaping the metabolic landscape of ecosystems by providing electron donors/acceptors or raw materials (Novikov & Copley 2013) that organisms assimilate to create metalloenzymes. Mineral informatics methods may be able to elucidate connections between minerals and biology. If minerals are found to be critical in shaping which metabolisms

occur/do not occur in certain environments, this may allow for the prediction of metabolisms in terrestrial and extraterrestrial environments for which we have mineralogical data.

v. What role did minerals play in the origin of life?

Several studies have posited that minerals played a critical role at the emergence of life on Earth, whether by influencing the homochirality of organic molecules or performing redox transformations and carbon fixation (Hazen & Scholl 2003; Hazen 2005; Hazen & Sverjensky 2010; Nitschke et al. 2013; Russell et al. 2018). Others have suggested that clays and other minerals with layered structures may have been the first self-replicating entities (Cairns-Smith & Hartmann 1986; Cairns-Smith 1990; Greenwell & Coveney, 2006; Brack 2013), though these hypotheses have not been confirmed experimentally (Bullard et al., 2007; Krivovichev et al., 2012). Mineral informatics, combined with phylogenetics, geology, and laboratory experiments, could be informative for deducing the likely role(s) that minerals played at the origin of life in Earth's deep past. If certain minerals are found to be uniquely critical to the emergence of life on Earth, this would have profound implications for the emergence of life on other planetary bodies where those minerals may or may not occur. The origin of life from a non-living substance involves considerable jump in the informational (static) complexity of the underlying molecular

structures, which should be taken into account in any possible scenario of molecular (r)evolution that led to the appearance of self-replicating living entities. The sudden rise in structural complexity corresponds to the drop in configurational entropy (Krivovichev, 2016). Can the (local) entropic changes associated with the origin of life be measured quantitatively and understood using mineral informatics data?

vi. **Can mineral networks serve as a planetary-scale biosignature?**

Roughly half of all known minerals are mediated by biology and 34% are exclusively biotic (Hazen & Morrison 2022; Hazen et al. 2021a; Morrison et al. 2021). Many of these minerals are formed when life opens up a new compositional space for the planet, such as the Great Oxidation Event (Hazen et al. 2008; Sverjensky & Lee 2010). However, some of this biogenic chemical space may be abiotically accessed on other worlds. Abundant atmospheric O_2, for instance, may be abiotically generated by various star–planet interactions (Meadows et al. 2018 and references therein). Earth and planetary mineral network analysis may reveal whether mineral networks of environmental, biological, geochemical, and mineralogical attributes can distinguish living from nonliving worlds.

vii. **Can mineral networks serve as a proxy for the extent of planetary evolution?**

Mineralogical evolution occurs when processes create new pressure–temperature–compositional regimes where solids can form (Hazen et al. 2008; Cleland et al. 2021; Hazen et al. 2021a; Hazen & Morrison 2020). Each stage of mineral evolution expands the network of mineralogy through the introduction of new minerals, localities, and paragenetic modes. The network of martian mineralogy, therefore, is thought to be a subset of the network of Earth's mineralogy, due to the halting or slowing of mineral-generating geological processes on Mars. One can consider Mars and Earth to be two points along a spectrum of terrestrial worlds whose geological (and biological) activities have differed in temporal extent. A hypothetical world where plate tectonics was sustained for ~1 Gyr but then ceased should have a mineral network that surpasses Mars's mineral diversity, but is still a subset of Earth's. In this way, mineral informatics helps us interpret the extent of a planet's mineralogical network as a record of ancient and extinct processes, revealing a planet's geological history.

When considering exoplanetary systems where element ratios (e.g., C:O or Mg:Si) differ greatly from those of our own solar system, this linear spectrum on which Mars and Earth lie becomes a multidimensional phase space (Unterborn et al. 2016; Unterborn and Panero 2019; Hinkel and Unterborn 2018; Putrika et al. 2021). Understanding mineral networks

from an informatics point of view may help to predict how planetary mineralogy might evolve in vastly different geochemical contexts.

viii. **Did the emergence and evolution of life play a role in the increase of average mineral structural complexity on Earth through deep time?**

It has been shown that complexity of Earth's mineral kingdom increased gradually during planetary evolution (Krivovichev et al., 2018), but it is unclear whether this trend is related to the increase in complexity in the course of biological evolution. The average structural complexity of minerals on the abiotic moon, for example, does not follow the same trend of increasing complexity through time. Minerals are relatively less complex than biological organisms, both in terms of their static (Krivovichev 2013, 2015) and functional (Hazen et al., 2007) complexities. However, Since life and the mineral kingdom co-evolved, the character of the evolution of mineral complexity on Earth (Krivovichev et al., 2018) may have been influenced by biological activity, and is thereby a potential bio-signature.

b. Successful Use Cases in Mineral Informatics

i. **The evolution of mineralizing environments, as characterized by their myriad, complex attributes**

Mineralization, and associated formational environments, vary significantly across Earth and neighboring planetary bodies, as well as

throughout the different historical stages of planetary evolution. These stages and environmental parameters dictate the types of mineralization that occur and, likewise, leave their mark in the complex chemical and physical attributes of the resulting mineral specimens. Understanding the changing characteristics of mineralizing environments spatially and temporally across our planetary systems requires the examination of huge volumes of mineralogical information. The beginning steps of this work included a survey of all formational environments of ~5700 known mineral species, resulting in a compiled dataset ripe for exploration (Hazen and Morrison 2022; Hazen et al., 2022). Initial exploration has led to the discovery that (1) 80% of all mineral species formed through processes that involved water; (2) 50% of minerals formed through processes directly or indirectly related to biology, with 34% of minerals forming exclusively through biotic processes; (3) 42% of minerals contain one or more rare elements (e.g., REE, PGE, As, Mo, Sn), elements which all together represent only 0.01% of crustal atoms; and (4) most minerals have only one (59%) or two (24%) modes of formation, with a few notable exceptions, including pyrite with the most modes of formation at 21 (Hazen and Morrison 2022).

An additional component of this work involves analyzing those myriad attributes of mineral specimens via cluster analysis to relate their complex

characteristics to their modes of formation, thereby determining the natural kind clustering of these mineral systems. There are many such projects underway, including those examining the formation of pyrite (Gregory et al. 2019; Zhang et al., 2019), garnet minerals (Chiama et al., 2020; 2022a; 2022b(in prep)), spinel oxide phases (Hindrichs et al., 2022), and presolar SiC (Boujibar et al., 2021; Hystad et al. 2021). Boujibar et al. (2021) performed cluster analysis on a range of isotopic data from presolar SiC grains in order to examine and compare the origins of these materials. This study made several exciting discoveries - while the clustering model agreed with previously defined grain types and origins in several aspects, there were notable and important deviations, including: a division of one grain type into three distinct types based on varying metallicity of the parent star, the arbitrary nature of certain divisions in systems that are continuous rather than discrete, the observation that asymptotic giant branch (AGB) stars with narrow ranges of mass and metallicity tend to have enhanced production of SiC, and enrichment in ^{15}N and ^{26}Al that is not explained by existing AGB models.

Next steps: This exploration of mineralizing environments and their characteristics not only provides an opportunity to integrate data from heterogeneous sources and types (e.g., X-ray diffraction, electron microprobe analysis, inductively coupled plasma mass spectrometry), but

also to link data from different fields of science to better understand mineral paragenesis. Handling heterogeneous data is a challenge (Reichman et al. 2011; Wang 2017) and many researchers have been actively working on using heterogeneous data for their analysis by creating methods, approaches, and pipelines to seamlessly clean, integrate, process, and analyze data (Wang 2017; Zhang et al. 2018; Beneventano & Bergamaschi 2004; Wiederhold 1999; Nazabal 2020). Additionally, the exploration conducted by Boujibar et al. (2021), provided another use case to test out machine learning methods on sparse data sets, thereby aiding in the eventual development of a sparse data framework (see Section 5a for more details).

ii. Mineral association analysis

Prediction of the locations of as yet undiscovered mineral deposits has long been a point of great scientific and economic interest. Mineralization and mineral co-occurrence across the varied geologic terrains of Earth and other planetary bodies has a level of complexity that makes prediction of mineral locations, or even the mineral inventory at a locality of interest, difficult. However, recent advances in the mineral locality data resources (e.g., mindat.org and the Mineral Evolution Database) have provided an opportunity to begin tackling this tough problem with machine learning. Association analysis can be used to create a recommender system (Burke

et al. 2011; Shah et al. 2017) that generates association rules based on known co-occurrences and these rules can be queried to determine the likelihood of currently unknown co-occurrences. In the case of minerals, we can query our mineral association rules to predict: A) previously unknown locations of a mineral species, B) previously unknown locations of mineral assemblages, including those that represent analog environments for study, and C) the mineral inventory at a locality of scientific interest. The mindat.org team have conducted preliminary explorations using pairwise associations to predict the occurrence of certain minerals on Earth.

Next Steps: Mineral association analysis provides new types of data problems. We need to modify the association analysis algorithms to better handle larger mineral occurrence datasets. For example, our models can currently handle only 2,473 minerals occurring in 87,306 localities (Prabhu et al. 2019; Morrison et al. 2022 (in prep)), but there are at present ~5760 mineral species in the International Mineralogical Association's (IMA) list of approved mineral species (https://rruff.info/ima/), which occur in more than 375,000 localities (https://www.mindat.org/stats.php). In addition to improving the scalability of association analysis methods, we also need to work on the dimensionality and reducing the minimum support of our method. For example, our method currently develops rules containing 4

minerals at a time, but there are localities with more than 50 coexisting minerals. Therefore, an important next step in our research is to increase the dimensionality of the association analysis method to handle more complex mineral assemblages. We also need to adapt our methods to enable inclusion of rarer mineral species that are known to occur in 17 or fewer localities (Prabhu et al. 2019). Lastly, we are currently developing a new approach to evaluate association rule mining methods (Prabhu et al. 2021b).

iii. Martian crystal chemistry

The scientific payload onboard the NASA Mars Science Laboratory (MSL) rover, *Curiosity*, is the one of the most advanced instrument suites ever landed on another planet. Part of this payload is the CheMin X-ray diffraction (XRD) instrument, which is used to characterize the mineralogy of rock and soil samples. CheMin is capable of identifying mineral phases present in samples, as well as their abundances and, for phases with an abundance ≥ 1–3 wt %, their unit-cell parameters. While there are instruments that analyze the bulk composition of martian samples, there is no instrument that directly measures the chemical composition of these mineral phases. However, in compiling data resources on mineral unit-cell parameters and compositions measured on Earth, the CheMin XRD patterns and resulting mineralogical data are used to predict the

composition of the mineral phases observed on the martian surface (Morrison et al. 2018a-b).

These initial studies, as those predating it, used unit-cell parameters to predict mineral composition in chemically limited systems, generally 2- or 3-element systems such as Fe-Mg olivine or Mg-Fe-Ca pyroxene (Morrison et al. 2018a-b). This limitation was due to the complexity of the compositional and structural parameter space when for or more elements are considered together. One way to develop a model that accounts for the complexity associated with multi-component systems and predicts the chemical composition of crystalline phases based on their crystallographic parameters is by using Label Distribution Learning (LDL) (Geng et al. 2013, 2014; Geng 2016). LDL is a machine learning algorithm originally created for facial recognition applications. When the approach was adapted for application to crystallographic and chemical parameters, it resulted in a model that accurately predicted the multi-component chemical compositions (up to 12 elements, in some mineral systems) of samples based solely on their unit-cell parameters (Morrison et al. 2018c). This crystal-chemical method has expanded the capability of XRD on spacecraft to that of a powerful chemical analysis tool, such as an electron microprobe, and has dramatically deepened our understanding of the geologic history of Mars.

Next steps: This exploration was the initial inspiration that motivated us to create a framework for small and sparse data (See section 6.a. for more details). In addition to our work developing a framework for small and sparse data, we will also need to develop methods to evaluate the accuracy of predictions made by our data models. This evaluation will attempt to address sources of uncertainty and how that affects our predictions. The LDL evaluation method being developed will address uncertainty of measurement (instrument errors), uncertainty from sampling (various sampling strategies to train predictive models), and most interestingly, scope compliance (Klas 2018) of the LDL method.

iv. Machine Learning Majorite Barometer

Diamond-hosted majoritic garnet inclusions provide important insights in processes that occur in Earth's deep mantle. Majoritic garnets provide the most accurate estimates for diamond formation pressures because laboratory experiments have shown that garnet chemistry varies as a function of pressure (Thomson et al. 2021; Akaogi & Akimoto 1977; Irifune 1987; Collerson et al., 2010; Wijbrans et al., 2016; Beyer et al., 2017). Thomson et al. (2021) show that none of the available barometers in the literature reliably reproduce the pressures of experimentally synthesized majoritic garnet over the entire pressure-temperature-composition space

549 investigated. Hence, they developed a barometer built using machine
550 learning algorithms (specifically random forest regression) and
551 experimental training data. This machine learning approach, tested with
552 various cross-validation methods, produces a barometer with a much
553 improved fit to the experimental data, especially at the highest pressures
554 and at extremes of composition space, and thus provides more reliable
555 estimates of formation pressures of diamond-hosted majoritic inclusions.
556 Applying the machine learning barometer to the global database of
557 diamond-hosted inclusions reveals that their formation occurs over
558 specific depth intervals that can be related to melting and decarbonation
559 of subducted oceanic crust.
560
561 Next Steps: While the machine learning approach improved the fit to the
562 available experimental data, it also revealed regions in pressure,
563 temperature, and most critically, composition space where the
564 experimental data set is sparse. Because many of the mineral inclusions
565 have compositions lying near or within sparse data regions, uncertainty
566 remains as to whether the barometer is accurately capturing their pressure
567 (and depth) of origin. Experiments can now be targeted to these specific
568 P-T-X regimes for an even more improved barometer. Machine learning
569 methods also can be used to predict the compositional variables that
570 correlate most strongly with changes in pressure, leading to an improved

crystal chemical and thermodynamic understanding of pressure-sensitive substitutions in garnet. These methods can also be applied to other mineral thermometers and barometers where large experimental datasets are fitted to extract thermodynamic solution parameters.

v. Comparison of mineral and protein metal clusters

Understanding the evolutionary stages of biology on a geological timescale is hampered by the propensity of organic matter to degrade within thousands of years without leaving physical fossil records. To understand how life evolved over the course of billions of years, proxy data are required.

At least five observations suggest that minerals can act as a source of proxy data from which to infer how biology evolved: 1) biology and geology are intimately connected, for instance, cellular organisms excrete minerals as metabolic end products (hazenite; Yang et al. 2011; greigite; Gorlas et al. 2018) and cellular organisms transmit electrons to and from minerals (Shi et. al. 2016), 2) cellular organisms and minerals use transition metals (Fe, Mn, Co, Mo, Cu, V, W, Ni) to perform electron transfer reactions, 3) mineral surfaces are hypothesized and shown to be capable of prebiotic reactions similar to those that extant proteins perform (Wachtershauser 1988, Novikov & Copley 2013), 4) minerals are similar to the rings of a tree in that

593 they provide information (e.g., temperature, humidity, etc.) about the
594 environment of formation, and 5) metal cluster structures of extant
595 proteins were observed to be so similar to the structure of bulk mineral
596 metal clusters as to be considered vestiges of minerals that were co-opted
597 and assimilated into biological systems (Russell & Hall 1997, Nitschke et al.
598 2013, Zhao et al. 2020).
599
600 Access to large mineral and protein structure databases allows the
601 potential to understand how mineral and protein metal clusters are
602 connected. Connecting the mineral world with biology will allow a deeper
603 understanding of how geology and biology co-evolved. Directly quantifying
604 metal cluster similarity between minerals and proteins is a challenge due
605 to comparing the finite protein cluster to a periodic lattice of a mineral.
606 Solutions using graph-based methods have been proposed (Zhao et al.
607 2020; McGuinness et al. 2022 (in review)). Each solution compared
608 subgraphs of mineral and protein metal clusters, however without
609 including metal coordination, and mineral dimensionality (2D-layer vs 3D
610 lattice) metal clusters were quantified as being highly similar (Zhao et al.
611 2020). Subsequent studies, building off the quantitative pioneering work
612 of Zhao et al., included these chemically important characteristics and
613 found FeS minerals and protein were significantly less similar (McGuinness
614 et al. 2022 (in review)) than previously proposed (Russell & Hall 1997,

615 Nitschke et al. 2013) Even though McGuinness et al. 2022 show that FeS
616 mineral lattices and protein metal clusters are not structurally similar, this
617 method has not been applied to other metal types such as Ni or Cu.
618 Applying the method developed by McGuinness et al. 2022 to additional
619 metal types may help understand the extent to which proteins and
620 minerals co-evolved as cellular metabolism and minerals became more
621 complex (Moore et al. 2017; Krivovichev et al. 2018).
622
623 Next Steps: An additional step towards a potentially more clear
624 understanding of how minerals and proteins are related is to compare
625 mineral surface and protein metal cluster structures. Mineral surfaces
626 expose the chemically active components that may have catalyzed
627 biologically relevant products under hydrothermal conditions on early
628 Earth (Novikov & Copley 2013). Comparing the surface properties of
629 minerals to the chemical properties of protein metal clusters might
630 elucidate the extent to which minerals acted as primitive enzymes at the
631 dawn of life. Did biology co-opt the chemical configuration of the
632 chemically active surface of minerals to reproduce the reactions that were
633 possible abiotically? Or did biology incorporate and reconfigure metal
634 building blocks (e.g., 2Fe2S) to meet growing cellular needs? Answering
635 these questions is challenging because mineral surfaces are complex,
636 subject to relaxation, are chemically active, display complexly irregular

surface topologies, and are affected by many solution conditions (pH, salinity, temperature, etc.) Alternatively, there also exists the possibility that protein metal clusters do not bear any significant resemblance to minerals (neither surface, nor lattice structure), suggesting an alternative pathway and relationship between mineralogy and biology in which biology acts independently, only relying on minerals for the feedstock (i.e., metals) to nucleate the information-rich systems that remain far from equilibrium.

5. Mineral Information Systems

a. A non-exhaustive list of open access mineral data resources

The mineral data resources we have chosen to highlight below are open and among the most widely used in the community. There are many other useful and important mineral data resources that are not yet available as open resources.

i. **International Mineralogical Association** (IMA) list of approved minerals (https://rruff.info/ima/) - a searchable database of mineral species information, including chemical formula, unit-cell parameters, paragenetic modes, and links to other important mineralogical data resources (e.g., American Mineralogist Crystal Structure Database, mindat.org, Mineral Evolution Database, Handbook of Mineralogy)

ii. **The RRUFF Project** (https://rruff.info/) - a mineral library and database of chemical, spectral, and diffraction data for mineral species (Lafuente et al. 2015).

iii. **The Mineral Evolution Database** (MED; https://rruff.info/Evolution/) - a database of mineral locality and age information, with ~200,000 species/locality/age records extracted primarily from scientific literature and mindat.org. (Golden et al. 2016; Golden 2019)

iv. **The American Mineralogist Crystal Structure Database** (AMCSD; http://rruff.geo.arizona.edu/AMS/amcsd.php) - a crystal structure database that includes every structure published in the *American Mineralogist*, *The Canadian Mineralogist*, *European Journal of Mineralogy*, and *Physics and Chemistry of Minerals*, as well as selected datasets from other journals.

v. **The Handbook of Mineralogy** - a five volume set with each of the 4988 pages dedicated to a mineral species description, with information such as crystallographic and physical attributes, microprobe chemical analyses, paragenetic mode and locality information, and select references.

vi. **Mindat.org** - the world's largest open database of minerals, rocks, meteorites and the localities from which they were found.[2]

[2] https://www.mindat.org/

vii. **Mineral Properties Database** (MPD; https://odr.io/MPD) - a database of various mineral attributes including age, color, redox state, structural complexity, and method of discovery.

viii. **Evolutionary System of Mineralogy Database** (ESMD; https://odr.io/esmd) - a database containing measured geochemical and physical characteristics of mineral samples, including major, minor, trace elements as well as isotopic ratios. (Chiama et al. 2022a)

ix. **The CheMin Database** (https://odr.io/chemin) - a database containing the X-ray diffraction data from martian rock and soil samples analyzed by the CheMin instrument onboard the NASA Mars Science Laboratory.

x. **The Astromaterials Data System** (AstroMat; https://www.astromat.org/) - a data infrastructure that stores, curates, and provides access to laboratory data acquired on samples curated in the NASA Johnson Space Center Astromaterials Collection, including the Apollo lunar samples and the Antarctic meteorite collection (Lehnert et al. 2019).

xi. **EarthChem** (https://earthchem.org/) - a data system providing open data services to the geochemical, petrological, mineralogical, and related communities, including data preservation, discovery, access, and visualization.

xii. **GEOROC** (Geochemistry of Rocks of the Oceans and Continents; http://georoc.mpch-mainz.gwdg.de/georoc/) - a global geochemical

699 database containing published chemical and isotopic data as well as
700 extensive metadata for rocks, minerals and melt/fluid inclusions.
701 xiii. **MetPetDB** (https://tw.rpi.edu/project/MetPetDB) - a relational database
702 and repository for global geochemical data on and images collected from
703 metamorphic rocks from the earth's crust.
704 xiv. **The Planetary Data System** (PDS; https://pds.nasa.gov/) - a long-term
705 archive of digital data products returned from NASA's planetary missions,
706 and from other kinds of flight and ground-based data acquisitions,
707 including laboratory experiments.
708 xv. **Mineral RI** (https://odr.io/mineralRI): a database containing the refractive
709 indices minerals and synthetic compounds. (Shannon et al. 2017).
710
711 b. Mineral Information Models
712 The global research community of mineralogy has made impressive progress on
713 information models for database construction and data sharing in the past
714 decades. From the point of view of data management, a good information model
715 should be correct, complete, and consistent. An effective way for information
716 modeling in real-world practice is to follow or adapt existing community
717 agreements or standards on mineralogy, such as those on the physical, chemical,
718 and biological characteristics of minerals. For instance, the Database of Mineral
719 Properties (https://rruff.info/ima/) maintained by the International Mineralogical
720 Association (IMA) keeps an up-to-date list of mineral species. The main

components in the information model include mineral name, chemistry, mineral groups, origins, paragenetic mode, IMA status, relevant references, and links to external sources such as mindat.org, Google Images, and Wikipedia.

As open data and data-driven studies are increasingly accepted in the geoscience community, many databases in the field of mineralogy also increase the visibility of their information model and build machine interfaces for data query, access, and download. For instance, the RRUFF database (https://rruff.info) has integrated records of Raman spectra, X-ray diffraction, and chemistry data for minerals. The user interface enables data query through mineral name and chemistry includes/excludes. Interested users can also contact the database manager for batch data download and sharing. Mindat.org (https://www.mindat.org) is another widely used database in the field of mineralogy. Its construction and maintenance follow a crowd-sourcing style. Besides the physical and chemical attributes of mineral species, a unique attribute on mindat.org is a comprehensive list of the localities where that mineral species has been found. In the past years, many research activities benefited from the open data shared by mindat.org. As each of those open databases has its own focus and information model, scientists in large-scale research activities often need to collect data from multiple sources. Recently, researchers in geoinformatics and data science also discussed the need for a more comprehensive mineral information model to document the extensive facets of

743 mineral data, such as the global earth mineral inventory (GEMI) proposed by
744 Prabhu et al. (2021a). Complementing these efforts are initiatives using semantic
745 technologies to build knowledge graphs for mineral species, as a preparation to
746 explore new ways for annotating and discovering mineral data shared on the
747 Internet (Brodaric and Richard, 2020).
748
749 The FAIR (findable, accessible, interoperable, and accessible) data principles
750 (Wilkinson et al. 2016) are now widely accepted in geoscience. Information
751 models are an important part of FAIR data. More community efforts, such as
752 through IMA, the Mineralogical Society of America (MSA), and the
753 Geoinformation Committee of the International Union of Geological Sciences
754 (IUGS-CGI), are needed to promote the quality and usefulness of the model
755 outputs.
756
757
758 6. Informatics Innovations Needed for Mineralogy.
759
760 The previous sections of this paper (and many other informatics papers focusing on
761 various domains) have clearly emphasized the value that informatics methods provide to
762 their respective domains (Lord et al. 2004; Goble & Stevens 2008; Heberling et al. 2021;
763 Collen 1986; Gauthier et al. 2019). However, a point often missed or overlooked in
764 scientific literature discussions is that innovations in data science and informatics are

usually driven by diverse datasets available in various domains and the needs of the use-cases utilizing those datasets. In this section we discuss some of the interesting data science challenges we observed while working with mineral data to try to answer some of the unanswered questions in geoscience.

Mineral data provide interesting and unique problems that limit the usability of existing machine learning methods meant to extract meaningful information from data.

a. Small and Sparse Data Framework:

   It has been widely publicized that we live in the "Age of Big Data" (Lohr 2012; Wise & Shaffer 2015; Yu 2016; Wachter 2019; Borgman et al. 2008), and understandably there has been a lot of research done into scaling-up algorithms, methods, software, and hardware needed to enable the exploration and use of very large datasets to gain valuable information. This focus has led to the creation and constant improvement of "big data frameworks", which provide a roadmap on how to work with large datasets. However, mineralogy, along with many other fields in Earth and planetary sciences, provide a plethora of small and sparse datasets that do not fall into the realm of big data. These datasets therefore require the application of methodologies that lie outside the focus of traditional big data researchers. The next major hurdle for mineral informatics (and geoinformatics in general) is to work towards creating a framework for small and sparse data.

For example, mineral data collected by the CheMin X-ray diffractometer onboard the Mars Science Laboratory (Morrison et al. 2018a; Rampe et al. 2018) has few data points, having analyzed ~40 samples, each with around a dozen mineral species (as of January 2022). The CheMin team used small (on the order of dozens to a few hundred data points) datasets of mineral composition and associated unit-cell parameters to build models capable of predicting the basic chemical composition of major mineral phases observed on Mars, based solely on their unit-cell parameters (Morrison et al. 2018a-b). However, the team wished to push their chemical prediction further - to predict complex, multi-element mineral compositions for the martian crystallographic data. In order to do so, Morrison et al. (2018c) assembled datasets of laboratory-analyzed complex, multi-element mineral compositions and unit-cell parameters, which contained only a few hundred data points for each of the major mineral groups identified by CheMin. Morrison et al. (2018c) used the small data Label Distribution Learning approach to predict complex chemical compositions (up to 12 elements, in some mineral systems) of mineral samples collected by the CheMin instrument based on the unit-cell parameters of these samples (See section 3b for more details). Significantly more work can be done here to increase the accuracy and performance of these models and such complex datasets with small sample sizes provide an interesting and rare challenge to data scientists.

Mineral geochemistry often contains information related to the geologic, chemical, and/or biological processes and materials that went into their formation and any subsequent weathering and alteration. However, geochemical data are inherently sparse due to chemical variability in geologic deposits and materials, different elemental affinities amongst different mineral species, and analytical bias introduced by research aims or instrument limitations. The resulting frequency of "missing values" makes many geochemical datasets unsuitable for use with existing algorithms designed for complete or near-complete datasets. A prime example of the sparseness of geochemical data is the garnet dataset compiled by Chiama et al. (2020, 2022b(in prep)), which contains over 95,000 geochemical analyses of garnet group mineral samples collected from a variety of sources, ranging from large repositories (EarthChem, RRUFF, MetPetDB) to individual peer-reviewed literature. Even a compiled and curated dataset such as this is considered sparse, largely due to the chemical variability amongst the various garnet mineral species, resulting in missing values in the chemical compositions of these samples (Chiama et al. 2022a). For example, of the 95,000 analyses compiled, only 5 major elements (Mg, Fe, Ca, Al, and Si) are present and/or reported in most samples, while other elements, including Mn, Cr, and Ti, are much less common throughout the dataset. An additional contribution to this sparseness is that studies may not analyze for all elements in a sample (e.g., limited to elements of interest, difficulty measuring light elements), resulting in missing values for which it is not known whether that element is present. Thus,

while analyzing these data (using descriptive, prescriptive, or predictive methods) we need to take into account these missing values and their effect on the results. Sparse data is not a problem new or unique to mineral data (Greenland et al. 2000; Greenland et al. 2016; Sweeting et al. 2004; Rogers et al. 2018), but, as is the theme for the rest of this paper, we must learn from the successes and failures of other domains in addressing sparse data (Shepperd & Cartwright 2001; Katz 1987; Uzuner 2009; Derczynski et al. 2013).

Other examples of small and sparse data challenges can be encountered in efforts to understand other planets and moons including Venus and Titan through their mineralogy and geochemistry. Frigid Titan's exotic mineralogy, with water ice as a principal rock-forming mineral, oceans of liquid hydrocarbons, and varied postulated organic minerals, is mostly understood through laboratory analogs (e.g., Fegley et al. 1992; Gilmore et al. 2017; Bullock & Grinspoon 1996; Hashimoto & Abe 2005; Treiman & Bullock 2012; Zolotov 2018; Hazen 2018; Maynard-Casely et al. 2018; Cable et al. 2021).

Small and sparse datasets are a common occurrence in Earth and planetary science. Despite the limitations of the available information, the answers to key scientific questions are tied to these datasets. Therefore, an effort to create a framework to handle small and/or sparse data will be highly beneficial to scientific research in Earth and planetary science. Many researchers are working on "High-

853 Dimensional, Small Sample Size" (HDSSS) or "High-Dimensional, Low Sample Size"
854 (HDLSS) and its use in data analytics (Liu et al. 2017; Golugula et al. 2011; Shen et
855 al. 2016; Yata and Aoshima 2012; Hall et al. 2005). However, this area of research
856 has received much less attention compared to its big data counterpart, and hence
857 has lacked the synthesis and generalization that comes with the popularity and
858 maturity of well-established fields. The aforementioned examples (including
859 section 3 and 5), clearly demonstrate how such a framework would open paths
860 for exploring very important scientific questions within and beyond mineralogy.
861
862 b. Data Discovery
863 An increasing trend of data science in recent years is doing research with open
864 data shared by others (Fox and Hendler, 2014). Several recent scientific advances
865 in mineral informatics also reflect that trend (e.g., Hazen et al., 2019). From the
866 point of view of data users, an ideal situation is that they can efficiently find data
867 portals on the Internet, datasets on the portals, or subsets of the data. In
868 comparison, from the point of view of data providers and data managers, they
869 need to organize the data with shared community standards, detailed metadata,
870 and persistent and stable facilities to increase the reusability. As illustrated in the
871 FAIR data principles for open data (Wilkinson et al., 2016), the first two key points
872 to consider are the findability and accessibility of data. Correspondingly, three key
873 technical items arise here. The first item is the metadata schema for describing
874 the datasets. While there are many common-purpose metadata schemas, such as

875 the Dublin Core, for describing datasets, for domain-specific data such as those in
876 mineralogy there can also be specific metadata elements. The second item is the
877 identifier for the datasets. Similar to the Digital Object Identifier (DOI) for
878 publications, datasets shared on the Internet should also have specific identifiers
879 to enable persistent and stable discoverability. The third item with respect to
880 findability and accessibility is the protocol for retrieving metadata through the
881 identifier of datasets. Community efforts such as DataCite (Brase, 2009) have
882 made solid progress toward that goal. Nevertheless, the wide implementation of
883 those best practices for open data in geosciences, including mineralogy, still need
884 more time. It is also important to remember that appropriate scientific credit must
885 be given at every stage of informatics methodology, from the acquisition of data,
886 to data analytics, and finally the dissemination of the research products produced
887 by the data analysis.
888
889 A very recent technical development regarding data discovery is the Dataset
890 Search Engine released by Google (Noy et al., 2019), which is able to index millions
891 of datasets on thousands of data portals, including their identifiers or Web links.
892 End users of the dataset search engine
893 (https://datasetsearch.research.google.com) have integrated access to thousands
894 of data portals. When a dataset is found on the engine, users can go to its original
895 data portal page through the identifier or Web link and then download. The
896 Google Dataset Search Engine is built on the top of Schema.org, which is designed

as a comprehensive metadata schema for annotating digital objects on the Web. The annotated objects, such as datasets, will then be indexed by the search engines. As its usage is expanding, Schema.org also provides space for extending the metadata elements of certain objects. A potential here is to have specific metadata elements designed for datasets of mineralogy, and this should be based on community collaboration. In the past few years, the EarthCube community has leveraged a list of open geoscience data portals to develop the GeoCODES search engine (McHenry et al., 2021). It is also based on Schema.org but has made extensions specifically for the registration and discovery of geoscience data. Any future efforts on the findability and accessibility of open mineralogy data can absolutely benefit from the technical structure and experience of GeoCODES. Community agreements and standards, such as those developed by IMA, MSA, and IUGS-CGI, as well as best practices in existing data portals, such as those in RRUFF and mindat.org, will also be helpful to enrich the metadata of open mineralogy data.

c. Data Processing

Dozens of data repositories contain a wealth of mineralogical information (see section 5a) from which large data resources can be extracted. Web-scraping algorithms allow for the retrieval and storage of large amounts of data from web sources (Glez-Peña et al. 2014; Zhao 2017). Scraping algorithms in scripting languages such as Python or R allow users to extract and compile large amounts

919 of data from web sources or journal articles in minutes or seconds, but the
920 structure (or lack thereof) of web pages can slow the production of new data
921 resources. Open-access mineral databases tend to be very contributor friendly;
922 thus, users can pick and choose which data to include for a particular entry.
923 Recognizing the inconsistencies in the storage and representation of mineral
924 attribute data within and across different mineralogical databases is essential
925 when compiling large mineral datasets from open data sources.

926 Webpages associated with Webmineral and Mindat have hierarchical structures
927 made up of Hypertext Markup Language (HTML), Extensible Markup Language
928 (XML), or Cascading Style Sheet (CSS) elements that allow for the selection of
929 nodes that can contain specific data a user is interested in (Gunawan et al., 2019).
930 The ubiquitous occurrence or rarity of mineral, relative interest among the
931 scientific community in a mineral, as well as the age of discovery cause significant
932 differences in the amount of information available for a mineral, driving the
933 differences in the structure of these webpages. Webpages and digital PDFs
934 associated with the *Handbook of Mineralogy* have very little structure, which
935 places more importance on the use of keywords (e.g., space group or crystal
936 system) or separators (e.g., each mineral attribute or property introduced may
937 have a semicolon preceding the associated description) in the compilation of data.
938 Nested conditional statements (i.e., if-else statements) are useful for compiling
939 data from web databases that have variable or no structure, but this approach can
940 be more time-consuming and prone to error. Some headers may be reused such

941 as “beta (ß)” which is used as a descriptor of the refractive indices in biaxial
942 minerals (e.g., Frazier et al., 1963; Gunter, 1992) and it can also refer to the
943 geometry of the unit-cell of dimensions (e.g., Grove and Hazen, 1974; Nesse,
944 1991).

945 d. Quantifying and Correcting Bias

946 Critical to all of these aspects of data resource development and use is an
947 understanding of and, where possible, modeling of the biases that exist in each of
948 these systems. For example, significant biases occur in mineral sampling based on
949 the physical appearance of the phase (e.g., large, brightly colored, euhedral
950 crystals), the economic value, the scientific interest, proximity to major
951 universities or research centers, and analytical technology. Such biases can be
952 corrected with models of each of these parameters (Hystad et al. 2019; Hazen et
953 al. 2016; Grew et al. 2017). Natural preservational biases is more complex, as it
954 involves geologic history and mineral properties (e.g., chemistry, solubility,
955 hardness), but work is underway to begin unraveling the history of preservational
956 biases in mineral systems on Earth and other planetary bodies (Liu et al. 2019).

957

958 7. Informatics research as a socio-technical system

959

960 Research in the field of informatics is heavily dependent on the interactions
961 between the data scientists and domain scientists (e.g., mineralogists, planetary
962 scientists) (Ma et al. 2017). Conducting and applying informatics research is very

much a socio-technical system (Herrmann 2011). It is as much about the researchers, their interactions, the hypotheses generated, and interpreting of results from visualizations or models as it is about the data, the algorithms, and the models. Collaborations in informatics include many iterations between data and domains scientists starting from data explorations and the problem formulation to interpreting the results and documenting the scientific insights learnt from the data.

We recommend starting an informatics exploration with an in-person or virtual "datathon" (Anslow et al. 2016; Fritz et al. 2020). During this datathon, which usually lasts a day or two, collaborators mainly focus on:

1. Interactions and discussions between data scientists and domain scientists to frame their goals and expectations.
2. Documenting the research questions to be explored.
3. Collating the data resources required to explore the documented research questions.
4. Exploring the methods needed to examine the data (both analytically and visually).
5. Constructing a roadmap for dividing the research question and tasks into smaller, more tractable parts.
6. Leveraging descriptive, prescriptive, and predictive methods to gain preliminary insights from the data.

7. Forming short term and long-term goals based on the preliminary results.
8. Documenting the shortcomings of the methods explored and why these roadblocks hamper scientific exploration.
9. Documenting the innovation needs of both data science and domain science methods to overcome the previously documented hurdles.

Not all of these steps need to be done during the two-day datathon; steps 1 and 2 can be completed beforehand. The main goal of conducting a datathon is to expedite and streamline the initial data exploration to gain preliminary results that can be examined by the domain scientist, while also allowing the data scientist to explore and understand the intricacies of the data at hand. Additionally, all collaborators gain an understanding of the shortcomings, needs, and opportunities of their data and of the current methods to address the desired scientific questions. This inventory of needs and opportunities in both the data science and domain science can result in a datathon output of a list of projects and publications spurred by the creative and iterative processes of this closely collaborative effort.

After the initial datathon, each collaborator (or group of collaborators) has a plan of action for the projects and subtasks within the project they are leading. Subsequent communication and collaboration usually follows the preferred working model of the team. For example, weekly meetings between the group to discuss advances in the project, or email communications between the team for

the same purpose. The steps taken after the datathon and methods to communicate and collaborate change depending on the work style and comfort levels of the collaborators. General recommendations for this step include "science of team science" best practices advocated by many communities (NASEM 2015).

8. Vision for the future

a. Implications

Durable and information-rich, minerals are the only ancient relics that offer direct, solid glimpses of eons of planetary transformation (Hazen 2021). It is important to extract the abundance of information contained in these mineral samples to improve our understanding of the evolution of our planet, our solar system, and the role our planet's evolving geosphere played in the origin and proliferation of life. Key, synergistic aspects of the ongoing paradigm shift in mineralogy includes systematic efforts to collect and curate mineralogical information in data resources that enable open and widespread dissemination, and the use of those data to make scientific discoveries.

b. Look around! (At other fields)

As mentioned earlier in this paper, informatics methods have been followed, implemented, and improved upon in other fields over the past decades. The concept of "X-informatics" has also been around since its first conceptualization in 2007 (Gray and Szalay 2007; Hey et al. 2009), and over the past decade there has been a steady decline in researchers conducting informatics research in the silos of their respective fields. When planning for a new paradigm like mineral informatics, it is important to learn from successes and failures of more mature fields of informatics (Lord et al. 2004; Goble & Stevens 2008; Heberling et al. 2021) and modify the methods developed by past researchers to apply them to comprehensively address our needs as a community.

Over the last decade, there have been some efforts at collating various data resources in the geosciences and providing these data to researchers with minimal barriers and maximum interoperability. These efforts include Onegeology (Jackson 2010), Onegeochemistry (Wyborn et al. 2021; Chamberlain et al. 2021), and Onestratigraphy (Wang et al. 2021). The Onegeochemistry initiative also includes plans to develop best practices for FAIR geochemical data, governance models to ensure participation and trust, and a business model to ensure long-term sustainability (https://www.earthchem.org/communities/onegeochemistry/). Efforts to improve the access, usage, and impact of mineral data resources can learn from the successes and challenges faced by such global initiatives. Developing a set of

best practices and recommendations for creating, linking, and releasing mineral data would improve the mineral data landscape and make it easier for researchers to produce and use mineral data without too many barriers.

Just as increasing the findability, accessibility, interoperability, reusability, and other important aspects of mineral data management and stewardship, obtaining scientific insights from mineral data using data-driven methods are another key facet of mineral informatics. For this, too, we can look to and learn from the success and failures of other domains applying informatics methods to answer their research questions. We hope the research directions for informatics and other fields like mineralogy, planetary science, and other related fields using mineral data that have been documented in this paper act as an initial step towards the ultimate goal of systematizing data driven scientific exploration using mineral data.

9. Conclusion

Mineralogy is facing new opportunities and challenges with the increased interest in and applications of data-driven methods. We believe the next paradigm for the field of mineralogy is that of mineral informatics. Mineral informatics focuses on deciphering the patterns and trends hidden in mineralogical, geochemical, and

related data and using these patterns to answer scientific questions, thus making important new discoveries. In this paper, we show how the study of minerals is essential to improving our understanding of the evolution of our planet, our solar system, and more. We present a broad methodology for the study and use of mineral informatics methods (Figure 1) and document the needs of the field and important scientific questions that may be answered using mineral informatics. We reiterate the symbiotic relationship between data scientists and domain scientists (e.g., mineralogists, planetary scientists, biologists) to make continuous and sustainable scientific progress.

In summary, our vision for the next decade of mineralogical research is built upon the systematic and coordinated study of mineral data and of the data science methods used to gain scientific insights.

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