**Background.** The study of planetary interiors is paramount in understanding and providing a unifying framework for a planet's formation, evolution into its present state, and past and present geophysical properties such as magnetic fields and atmospheric conditions. In this era of prolific exoplanet discovery, the quest to investigate planetary interiors and surface conditions is more pressing than ever. With the growing number of exoplanets ranging in size from super-Earths to sub-Neptunes, and the omnipresent goal of "finding a new Earth", it is becoming evident we need to concentrate our studies on such planets. Currently, radial velocity and transit methods used to detect exoplanets give mass and radius data for exoplanets but offer no compositional information. Comparing the mass and radii of exoplanets with mass-radius relationships of pure materials such as iron, silicates, and ice, and stoichiometric mixture thereof, offer a glimpse into their plausible bulk compositions [2-4]. However, attempts to infer bulk composition have resulted in degeneracy with many interior composition combinations fitting mass and radius values for a particular exoplanet. Many models assume planets are fully differentiated, yet previous works using density functional molecular dynamics (DFT-MD) simulations at high pressures and temperatures have predicted deviations from this model. For example, the miscibility of $H_2O$ with H and He [5] and miscibility of Fe and MgO [6]. Contrary to traditional models, we infer "fuzzy layering" if material is miscible at boundary conditions, which would result in the gradual mixing of heavier elements into the upper, less dense layers. DFT-MD simulations are a powerful tool in predicting the equation of state (EOS) of a wide variety of planetary materials and mixtures at conditions that are difficult to achieve empirically.

**Hypothesis.** Some super-Earth and sub-Neptune exoplanets, termed waterworlds, contain a significant amount of water ($H_2O$) ice overlaying a magnesium silicate interior [7,8]. The stability of such a stratified internal structure depends on whether these simplified two-layer models reflect realistic water world structures. Instead of relying on static two-layered models, I am motivated to explore the dynamics of material mixing at the magnesium silicate-ice boundary layers under P-T conditions relevant to the interior conditions of waterworlds. Understanding whether these two materials are miscible will help us better resolve the internal composition and stratification of water worlds. **I propose to study the miscibility of a common high-pressure planetary magnesium silicate, enstatite ($MgSiO_3$) [9], and high-pressure water ($H_2O$) ice using DFT-MD.** $MgSiO_3$ will be referred to as rock and ice is assumed to be water ice for the remainder of this proposal.

**Research Plan.** (*Research Goal 1: Building Rock-Ice Systems and running DFT Simulations*) I will build the rock-ice systems and equilibrate each to a respective pressure in gigapascals (GPa) (**Table 1**).

***Table 1. Systems with $MgSiO_3$ and $H_2O$ crystal phases, space groups, and initial system pressure***

| System | $MgSiO_3$ phase | Space group ($MgSiO_3$) | $H_2O$ phase | Space group ($H_2O$) | P[GPa] | x |
|---|---|---|---|---|---|---|
| 1 | ppv | *Cmcm* [63] | ice X | *Pn-3m* [224] | 120 | 0.29 |
| 2 | pv | *Pnma* [62] | ice X | *Pn-3m* [224] | 60 | 0.29 |
| 3 | pv | *Pnma* [62] | ice VIII | *I41/amd* [141] | 30 | 0.26 |

The crystal phases chosen for each material present at 0K were the most stable structures at each respective pressure (**Table 1.**). I will run simulations on each system using a canonical ensemble (constant number of particles N, constant volume V, and constant temperature T) increasing the temperature of each system from 500 K to 8000 K with the Nosé-Hoover thermostat [10]. I will perform simulations in 500 K increments in a "heat-until-mixes" approach, similar to the "heat-until-melts" method [11]. Although this approach is prone to overestimating melting temperatures, my goal is to calculate the upper bound P-T conditions for rock-ice mixing which will be accomplished with my MD. I describe each system by its ice to rock mass ratio $[m_{H_2O}/(m_{H_2O} + m_{MgSiO_3})]$, for example, System 1 has an ice to rock mass ratio of 0.29. Then to investigate in which proportions rock and ice will mix I will simulate additional systems with ice

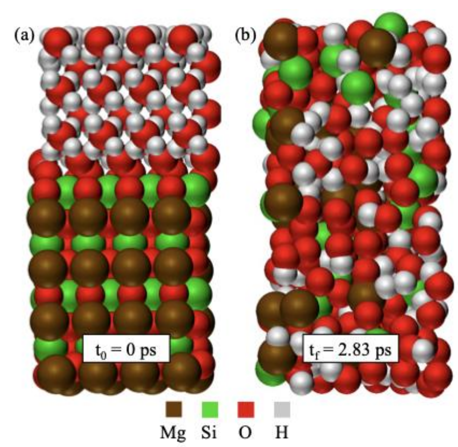

**Figure 1.** (a) initial configuration of System 1 and (b) final configuration with mixed rock and ice. MD simulation performed at 8000 K.

mass ratios of 0.29 and 0.20. I will accomplish this by increasing the number of rock molecules while keeping the number of ice molecules constant. If the two materials spontaneously mix during the simulations, I will know rock and ice are miscible at this temperature. Preliminary results from my MD simulations of System 1, run at 8000 K (**Fig 1.**) show exciting, novel results of miscibility.

(*Research Goal 2: Determining Miscibility*) An efficient way to detect mixing is to analyze how far atomic species move from their original positions by calculating their mean squared displacement (MSD). When the diffusion coefficient for all species is above zero, I will consider the system fluid. However, I will not know based on MSD alone whether the atoms crossed the rock-ice interface. The system could contain molten rock and water which remain immiscible instead of forming a homogeneous mixture. Therefore, I will also visualize each trajectory and verify that diffusion occurs across the boundary. My final method for confirming miscibility is to calculate the radial distribution functions (RDF) of magnesium (Mg) and silicon (Si) versus the oxygens (O) in $MgSiO_3$, termed rock oxygens, and oxygens associated with ice, termed ice oxygens. My goal is to show that Mg and Si lose coordination with the rock oxygens and interact with the ice oxygens. For example, when I plot Mg–$O_{rock}$ and Mg–$O_{ice}$, at the same temperature, if rock and ice are miscible, their radial distribution curves should overlap.

**Intellectual Merit.** In addition to working with my Ph.D. advisor, Dr. Burkhard Militzer at U.C. Berkeley, I will collaborate with Dr. Sarah Stewart, a professor in the Earth and Planetary Science Department at U.C. Davis, to perform dynamic smoothed particle hydrodynamic (SPH) simulations of colliding planetary bodies. This will give insight into whether these large impact events produce the conditions necessary for material mixing. It is important to determine post impact conditions because giant impacts govern an important stage of planet formation, mold their interiors, and drive geophysical properties [12].

Multicomponent EOSs of material mixing will shift the planetary science community's focus from static planetary models, where fully differentiated layers are modeled, to dynamic ones which include chemistry deep within the planet. If we neglect the presence of "fuzzy layers" within planets, we may miss key planetary properties such as its thermal evolution and magnetic field generation, which influence other properties such as tectonics, outgassing, dynamics, and volcanism. I plan to continue investigating rock-ice miscibility by considering other rocky material, such as $Mg_2SiO_4$ or MgO with $H_2O$, and exploring lower pressure regimes [8]. Moreover, provided that the necessary conditions are reached, I will further my research to elucidate whether a homogeneously mixed rock-ice layer could persist over long periods of time and even become stably stratified within water worlds. This will affect overall heat flow throughout the planet which will help us better understand the evolution of water worlds.

**Broader Impacts.** My proposal has applications in a diverse range of disciplines such as condensed matter physics, high energy density physics, geochemistry, and geophysics. I will publish my work in journals (e.g. PNAS), present at conferences (e.g. AGU and APS), and most importantly continue outreach by presenting my research at local, public seminars (e.g. BASIS, SLAM, and Compass Lectures). I spent my first summer as a graduate student volunteering at two workshops recruiting students to pursue graduate school in planetary science. I also began tutoring environmental sciences at San Quentin Prison which helps keep me informed on challenges facing our most at risk communities and how to aid in their success as aspiring geoscientists. After only one year in graduate school, I have already helped form the first Unlearning Racism in the Geosciences (URGE) pod at Berkeley. We will present our pod's work of integrating URGE deliverables into the Berkeley EPS department-level strategic plan for enhancing diversity at AGU 2021. The NSF fellowship will allow me to produce and share my findings with my peers as well as a general audience, increase equity in my field, and recruit the next generation of geoscientists.

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