ORIGINAL ARTICLE

The Homogeneous Mixing of MgO and H$_2$O at Extreme Conditions

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Abstract

Investigating water worlds presents a unique opportunity to understand the fundamental processes of planetary formation and evolution. One key aspect is characterizing the interactions between water and rock under the pressures and temperatures present within these worlds. In particular, investigating the conditions for the homogeneous mixing of these materials is imperative to characterizing bulk properties and evolution of water-rich exoplanets. **Here we use density functional molecular dynamics simulations to study MgO-H$_2$O mixtures at high pressure-temperature conditions where H$_2$O occurs in solid, superionic, or liquid form. MgO, the representative rocky material, can be either solid or liquid. We start from 500 K at 120 GPa, increasing the temperature step by step up to 8000 K. By inspection, we determine the temperature at which MgO-H$_2$O homogeneously mix in our simulations. At 6000 K and 174 GPa is when we find the system to homogeneously mix. This heat-until-it-mixes approach provides us with an upper bound on the temperature for the mixing of MgO and H$_2$O. We find that homogeneous mixing occurs at sufficiently low temperatures to be relevant for the collisional growth of a water-rich planet.**

KEYWORDS:
Planetary interiors, DFT-MD, High pressure, Water worlds, MgO, H$_2$O, Superionic ice

1 | INTRODUCTION

Water worlds are thought to have formed beyond the H$_2$O ice line, a region in the protoplanetary disk where water ice and rocky material are present in similar quantities. [1] Planetary system formation models suggest that these water-rich exoplanets migrated towards their sun resulting in close-in sub-Neptunes. [2,3] A simplified representation of the compositional profile of a water world typically consists of a central core made of metallic iron, a rocky mantle, a significant layer of water ice and in some cases, a water-rich gaseous envelope. [4,5] Studies have postulated that there could be rock-ice interactions in exoplanets that are water-rich or contain magma oceans, using the assumption that rock-ice mixtures would be found within these exoplanets at high pressures beyond a second critical point (SCP). [6,7] The SCP being the highest pressure and temperature at which two separate fluid phases can exist together, after which they mix and become a single fluid phase. Recent studies have shown that mixing of rocks and water ice is possible at extreme conditions. [8–10] It is important to consider that the high-pressure phase change of H$_2$O from the solid to superionic phase, which is well beyond the SCP, may lead to complex and unexpected rock-ice interactions. It is essential to determine the temperatures at which mixing occurs for other relevant planetary building blocks, such as MgO, as the presence of a mixed phase will have a considerable impact on the internal structure, density, and heat flow of water-rich exoplanets.

According to theoretical models, some close-in water worlds can have a high water content, with estimates of 37-50% of the planet's total mass being water.[11,12] Due to these massive water layers, the material at the rock-ice boundaries experience high pressures.[11] If the surface temperatures of these water worlds are high,[12] it is crucial to consider the possible mixing of materials at the rock-ice boundary. Even if a water world has fully differentiated, giant impacts during the growth process lead to the dynamical mixing of the layers and temperatures reach on the order of 10^4 K, resulting in a mixed mantle.[8]

In this study, we examine representative materials for a mixed rock-ice phase, specifically a mixture of MgO and H_2O created by the transformation process $MgO_{sol} + H_2O_{sol/superionic/liq} \rightarrow \left(MgO_2H_2\right)_{liq}$. Using first-principles simulations, we determine which phases are present in thermodynamic equilibrium. In general, a system composed of two distinct phases at a specific concentration is characterized by a phase boundary. If temperatures are low, homogeneous mixtures are unstable, and instead, the two materials are phase separated. The mixing of the two materials designates the pressure and temperature at which a single mixed phase becomes thermodynamically stable.

High pressure dynamics for rock and icy systems have been previously investigated.[8–10,13–20] However, it remains unclear how the binary phase diagram of MgO and H_2O evolves at the pressures and temperatures where complex MgO–H_2O phases decompose into constituent crystal phases MgO and H_2O. Therefore, we will assume that at the pressures under investigation, the MgO-H_2O system we plan to investigate has surpassed the SCP[15] and remains below where one would expect to find ultrahigh phases of MgO–H_2O compounds.[10] The SCP indicates the temperature and pressure at which two immiscible materials (liquid-liquid or solid-liquid) form homogeneous mixtures. Beginning at a pressure well beyond the SCP for rock-ice systems, as we increase the temperature, we expect to observe 3 phase changes in our binary system: a solid MgO + solid H_2O phase, followed by a solid-liquid phase, and ultimately the formation of a homogeneously mixed fluid (see Fig 4b in Ref.[15]). However, it is uncertain whether high-pressure phases such as superionic would result in additional dynamic interactions with MgO.

The mixing of MgO and H_2O has implications for the differentiation and thermal evolution of water-rich exoplanets. Relying on equations of state (EOS) of individual rocks and ices alone may not be sufficient to predict their behavior at conditions where mixing takes place and an EOS of the mixture would be more appropriate. The following results can serve as the basis for future explorations into the thermal evolution of water world interiors, by identifying the temperatures under which rock-ice dissolution is significant.

2 | SIMULATION METHODS

2.1 Preparation of Simulation cell

To begin, the cubic primitive cell for B1-MgO was replicated $2 \times 3 \times 3$ and relaxed to 120 GPa, resulting in cell dimensions $8.8742 \times 8.8742 \times 12.2689$ Å^3. The cubic ice-X primitive cell was replicated $3 \times 3 \times 3$ and similarly relaxed to 120 GPa resulting in cell dimensions $8.2011 \times 8.2011 \times 8.2011$ Å^3. These cells were strained in order to merge both structures into a periodic supercell with dimensions $8.5377 \times 8.5377 \times 20.4700$ Å^3, comprised of 48 MgO units in the B1 phase and 54 H_2O molecules in the ice X phase that were merged in the [001] direction (See figure 2A). It is worth noting that due to the inherent mismatch in lattice constants between the MgO and H_2O crystals, it was necessary to adjust the lattice constants of both structures to fit them into a single, periodic supercell. The change in lattice constant for each crystal was $\sim 3\%$. We relaxed the atomic positions in fixed cell geometry and then also relaxed cell vectors to achieve hydrostatic conditions at 120 GPa. This removed the residual stresses that resulted from the straining of the lattice constants and from merging the materials. Therefore, the intial MgO-H_2O supercell dimensions we began simulating with were $8.2886 \times 8.2886 \times 19.8728$ Å^3.

2.2 Heat-until-it-Mixes Simulations

We used density functional theory molecular dynamics (DFT-MD) simulations to determine the mixing of MgO (B1 phase) and H_2O (ice X phase) using a method called "heat-until-it-mixes," as previously described in Kovačević et. al.[8] This method involves conducting DFT-MD simulations at constant volume and incrementally increasing the temperature to determine at what temperature the two materials mix homogeneously. We increased the temperature by performing molecular dynamics simulations in increments of 500 K from 500 K to 8000 K. Mixing is determined by observing if the two materials spontaneously coalesce within a given simulation. The outcome of these simulations is an isochore in P−T space.

A method similar to this, the "heat-until-it-melts" method, overestimates melting temperatures due to the use of defect-free samples. However, the heat-until-it-mixes method should not lead to a significant overestimation in mixing temperatures because the presence of the rock-ice interface resembles the two-phase method,[21] which is an accurate method commonly used to calculate melting temperatures. In conclusion, this method provides a reasonable upper bound for the true mixing temperature.

The DFT simulations were performed using the Vienna Ab Initio Package (VASP) which uses projector augmented wave (PAW) pseudopotentials[22–24] and Perdew, Burke, Ernzerhof (PBE) functional.[25] A canonical ensemble (constant NVT) was used and temperature regulated with the Nose-Hoover thermostat.[26,27] Listed are the pseudopotentials used with valence states described with electron configurations as follows: Mg([Ne]$3s^2$), O([He]$2s^2 2p^4$), H(ultrasoft). All simulations used Γ-point sampling and a 900 eV cutoff energy for the plane wave expansion. A time step of 0.2 fs was used for all molecular dynamics. The results obtained were well converged with respect to energy cutoff and equilibrated for at least 4 ps.

3 | RESULTS

We investigated the mixing of MgO-H_2O under conditions relevant to the rock-water boundary within water worlds. Specifically, we focused on a single rock-ice system, where the density was held constant and we varied the temperature. We achieved this by increasing the temperature in 500 K increments from 500 to 8000 K. The results of our calculated pressure and internal energy, are presented in Table 1. Here we used this heat-until-it-mixes method to determine the temperature at which the two materials form a single homogeneous liquid. The stable phase at each P-T condition was determined by plotting the mean squared displacement (MSD) in the z-direction for each atomic species and plotting pair correlation functions of the magnesium ions relative to the oxygen atoms associated to rock and water.

The heat-until-it-mixes approach we use is expected to provide an upper bound for the mixing temperature.[8] The phases we observed in our simulations were solid MgO and solid H_2O (hexagon symbols in Fig 1). Then transitioned to MgO interfaced with superionic H_2O phase at ~ 1500 K ('×' symbols in 1). The superionic phase is characterized by the oxygen atoms remaining fixed in their lattice positions while the hydrogen atoms diffuse, in a fluid-like manner, throughout the oxygen lattice.[28] However, we did not observe any diffusion of hydrogen atoms through the solid MgO structure. Next was MgO and liquid H_2O (blue triangle symbols) at ~ 4500 K which is in agreement with the plotted H_2O melt curve.[29] The MgO crystal stayed in its solid phase until dissolving into H_2O and becoming a homogeneous liquid at ~ 6000 K, which is substantially below than the melting temperatures found for MgO.[30]

A direct method to detect the melting and mixing of materials is by tracking the movement of an atomic species throughout a trajectory via the mean squared displacement (MSD). If an atomic species diffuses, its MSD will increase linearly over time. **To get an indication of mixing, we track the MSD orthogonal to the rock-ice interface, or z-direction (Fig. 3A and 3B).** If the MSD of an atomic species increases with time it indicates diffusion and is evidence for mixing. At 4000 K, Fig. 3A, the H_2O is in a superionic state indicated by the hydrogen ions having an MSD that rapidly increases with respect to time. All other atomic species have an MSD that does not increase over time. However, there could be dissolution on timescales that DFT-MD cannot capture, and using the heat-until-it-mixes method can, at best, offer an upper bound for mixing. A more rigorous method, such as thermodynamic integration, may be used in the future to more accurately capture the mixing temperature.[31] Figure 3B clearly shows that the MSD's for all atomic species increase with time, which are rapidly diffusing. **Moreover, to demonstrate that our 6000 K simulation has reached convergence, we include Fig. 3C, which shows the total MSD in the 3 spacial dimensions. However,** MSD alone does not provide enough evidence for the dissolution of MgO into the H_2O. To verify whether the materials have mixed or if phase separation is still present, we will use pair distribution functions, $g(r)$.

Fig.4 shows the Mg-O_{rock} and Mg-O_{water} $g(r)$ functions for simulations where the temperatures were below mixing (4000 K) with dashed green and blue lines and above it (6000 K) with solid green and blue lines. The $g(r)_{Mg-O_{rock}}$ and $g(r)_{Mg-O_{water}}$, at larger r, remain phase separated at 4000 K which we can see in the deviation from unity. This behavior is not observed in simulations performed at 6000 K, which is above the mixing temperature for the MgO-H_2O system. This method allows us to simply identify the boundary between the unmixed and mixed phase regimes, as we show in Fig. 1.

Additional simulations were run to analyze uncertainty due to finite size effects. **We performed additional simulations of systems containing 96 MgO units and 90 H_2O molecules at similar pressure conditions and found that the system again mixes at 6000 K, which is consistent with the mixing conditions of the original cell size.**

4 | DISCUSSION & CONCLUSIONS

A recent study[8] provided theoretical evidence that energetic impacts of water-rich planets lead to the dynamic mixing of the rock and water resulting in a mixed rock-ice mantle. A sufficiently large mixed mantle would alter the dynamics and evolution of a water world. For example, as a rock-ice mixture cools, the thermal evolution of this homogeneous mixture remains unknown.

Table 1 EOS table of pressures and internal energies at temperatures simulated. The density of the simulation cell containing 258 atoms has a density of 4.1814 g/cc. The 'phase' column specifies the phase in which each material was during simulations, and the 'state' column indicates whether the two material remained phase separated or mixed.

Temperature (K)	Phase	State	Pressure (GPa)	Energy (Ha/cell)
500	MgO (solid) − H_2O (solid)	separate	121.94 ± 0.03	-41.44 ± 0.003
1000	MgO (solid) − H_2O (solid)	separate	124.46 ± 0.06	-40.28 ± 0.01
1500	MgO (solid) − H_2O (solid)	separate	127.91 ± 0.08	-39.46 ± 0.02
2000	MgO (solid) − H_2O (superionic)	separate	133.52 ± 0.12	-37.96 ± 0.03
2500	MgO (solid) − H_2O (superionic)	separate	138.68 ± 0.12	-36.33 ± 0.01
3000	MgO (solid) − H_2O (superionic)	separate	142.72 ± 0.21	-34.97 ± 0.02
3500	MgO (solid) − H_2O (superionic)	separate	146.26 ± 0.16	-33.79 ± 0.02
4000	MgO (solid) − H_2O (superionic)	separate	151.23 ± 0.16	-32.31 ± 0.04
4500	MgO (solid) − H_2O (liquid)	separate	155.97 ± 0.17	-30.84 ± 0.04
5000	MgO (solid) − H_2O (liquid)	separate	161.66 ± 0.36	-29.13 ± 0.08
5500	MgO (solid) − H_2O (liquid)	separate	168.45 ± 0.39	-27.14 ± 0.09
6000	MgO_2H_2 (liquid)	mixed	174.40 ± 0.21	-25.36 ± 0.04
6500	MgO_2H_2 (liquid)	mixed	179.40 ± 0.29	-23.81 ± 0.05
7000	MgO_2H_2 (liquid)	mixed	184.44 ± 0.20	-22.21 ± 0.04
7500	MgO_2H_2 (liquid)	mixed	189.01 ± 0.24	-20.77 ± 0.04
8000	MgO_2H_2 (liquid)	mixed	193.98 ± 0.30	-19.33 ± 0.06

This is significant for understanding the interior dynamics of water worlds, as recent experimental results have indirectly shown that MgO leaches from forsterite (Mg_2SiO_4) and dissolves into ionic water at high pressures and relatively low temperatures. It has also been shown that the electrical conductivity of molten MgO increases sufficiently to generate a magnetic field within super-Earths.[32] However, it is unknown whether a rock-ice mixture is electrically conductive enough to generate a magnetic field or if it would suppress any dynamo action. Through further modeling and experimentation on the properties of rock-ice mixtures, we can gain insight into water-rich planetary interiors.[7,33,34]

Rock-ice mixing also has implications for the formation of a secondary atmosphere of an exoplanet.[35,36] For example, a mixed rock-ice mantle could be a rich source for oxygen and hydrogen for the production of H_2O via outgassing for sub-Neptunes after the H_2O on the surface has been photoevaporated. Volcanism within the planet can release the trapped volatiles forming a high mean molecular weight secondary atmosphere.[37] An atmosphere with a high mean molecular weight includes water which has been recently discovered by the JWST mission in the atmosphere of WASP-39b.[38] The mixing of rocky material and ices has also gained interest as a possible hypothesis for the luminosity differences between Uranus and Neptune.[33]

Experimental techniques, such as the laser-heated diamond cell (LH-DAC) have provided valuable insights into the interactions between materials. However, to achieve accurate results, the samples used in these experiments must be able to withstand the rapid temperature changes that occur during quenching. The interaction between MgO and H_2O under high pressure and temperature conditions was recently studied,[9] but determining the amount of MgO dissolved in H_2O requires accurate solubility estimates based on the quenched sample. To overcome this limitation, using first-principle methods to simulate the interaction between MgO and H_2O in equilibrium allows us to reach extreme conditions and gain a deeper understanding of these interactions. The capacity for MgO to dissolve into H_2O and form a homogeneous liquid have important implications for the interiors of water worlds where these conditions exist. Our study provides an estimate of the temperature required to mix MgO and H_2O under such conditions. We suggest that future studies on the properties of water-rich exoplanets take into account the impacts of mixing and demixing on their thermal evolution, and consider non-ideal mixing effects.[39,40]

In our previous work,[8] we determined that $MgSiO_3$ and H_2O started to mix as soon as the temperature became sufficiently high for the $MgSiO_3$ phase to melt. Here we found, however, that MgO and H_2O began to mix at temperatures that were 2000 K below the melting line of MgO. This provides us with ample motivation to study the MgO-H_2O system further and provide similar tantalizing evidence that not all rocky materials behave the same at extreme conditions.
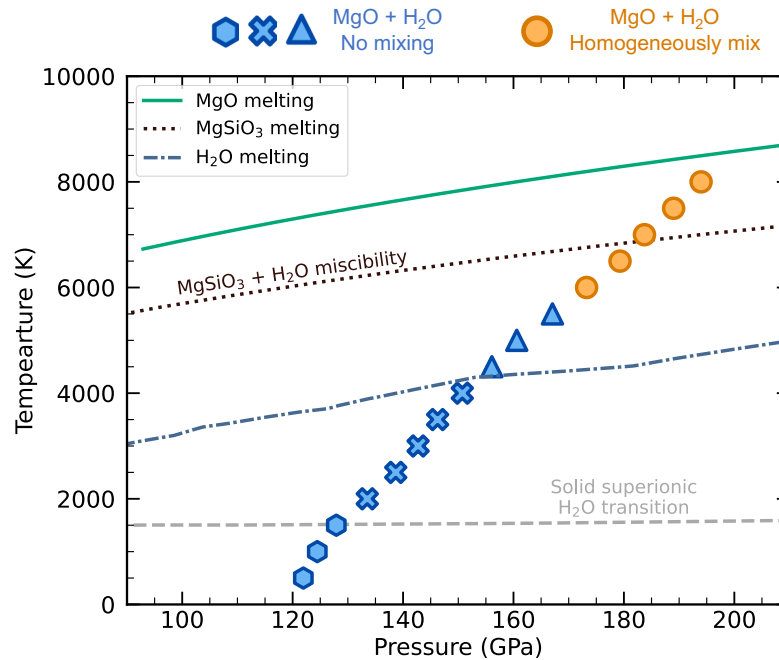
Figure 1 An isochore for the rock-ice system is plotted in *P-T* space. The blue symbols represent conditions under which rock and water remained separate, while the orange symbols indicate a fully mixed rock-water fluid. Our simulations predict that mixing occurs well below the MgO melt curve.[30] With increasing temperature, water transitions from a solid (blue hexagons) to a superionic phase (blue crosses) and finally liquid phase (blue triangles). The solid-to-superionic phase boundary[28] and H_2O melt curve[29] are plotted. For reference, the $MgSiO_3 - H_2O$ miscibility curve[8] is also plotted.

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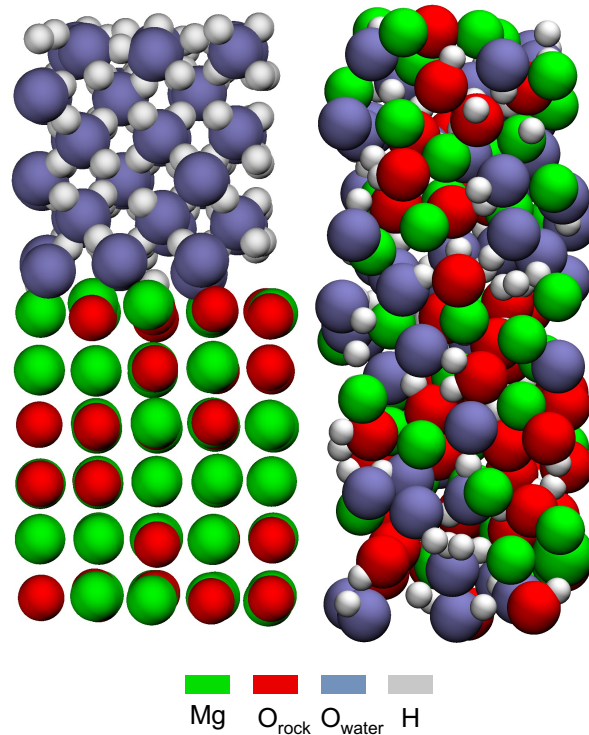
Figure 2 Simulation of the rock-ice system relaxed to 120 GPa (4.1814 g/cc). **(A)**: Initial configuration water (top) in the ice X phase and rock (bottom) in the B1 phase. **(B)**: Illustration of rocky-water mixing at T = 6000 K obtained after a simulation time of 8.3 ps. The atoms are colored by species: Mg (green), O_{rock} (red), O_{water} (purple), H (white).

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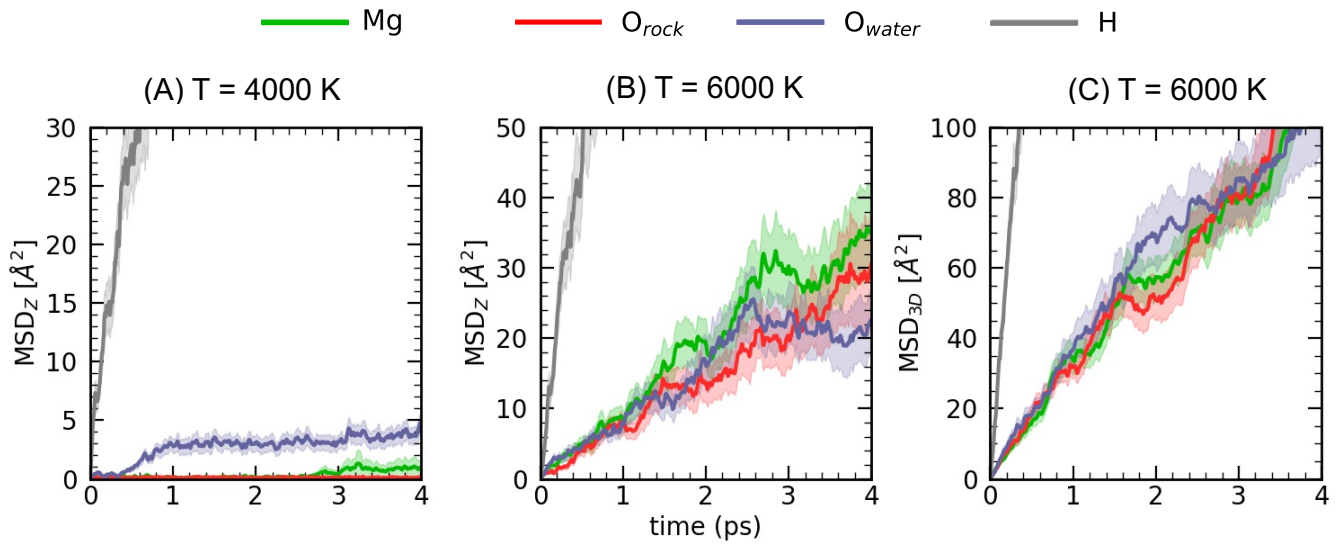
Figure 3 Mean squared displacement (MSD) and standard deviations for each atomic species at **(A)** at 4000 K where MgO remains solid and H_2O is superionic and **(B)** and **(C)** 6000 K where MgO and H_2O mix. MSD in the z-direction, or the direction orthogonal to the rock-ice interface, is shown in **(A)** and **(B)**, while MSD in 3D at 6000 K is shown in **(C)** to show that we have converged the simulation. Each line color on the plot corresponds to an atomic species: Mg (green), O_{rock} (red), O_{water} (purple), H (gray).
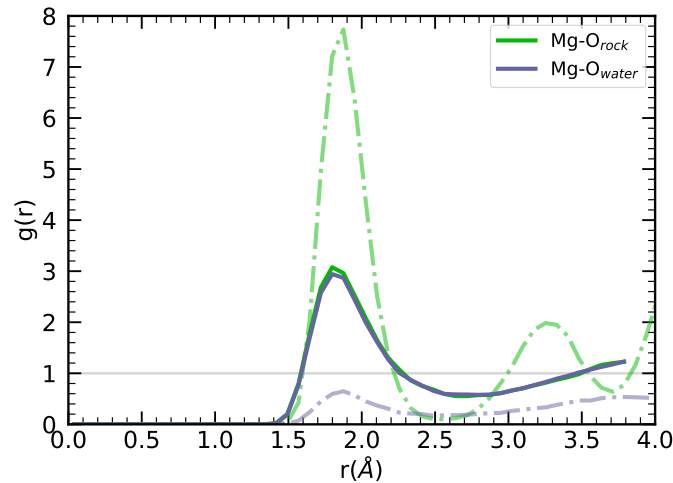

Figure 4 Pair correlation functions between magnesium and oxygen atoms in $Mg(O)_{rock}$ (green line) and in $H_2(O)_{water}$ (purple line). The dashed line corresponds to the unmixed system (4000 K) and the solid lines the homogeneously mixed system (6000 K). In the unmixed system (dashed lines), the pair correlations are less than one, indicating two separate phases. When the two phases mix homogeneously, the correlation functions become identical (solid lines) and asymptote to one at larger values of *r*.

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