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Inter-site Partitioning of Iron in Wadsleyite at High Pressures
ROSE PEREA, BORIS KIEFER, Department of Physics, New Mexico State University — $(Mg_{1-x},Fe_x)_2SiO_4$ – wadsleyite is thought to be the most abundant metal in the upper part of the Earth's transition zone (410 -520 km depth). Wadsleyite contains three crystallographically non-equivalent octahedral sites, M1, M2, and M3. Experimentally, it has been observed that the M2 site is depleted in iron relative to the M1 and M3 sites. This asymmetric partitioning may affect the melting temperature and the density of iron bearing wadsleyite and influence the transport of mass, momentum, and energy across the transition zone. We performed LDA and GGA first-principle calculations of ferrous iron substitutions in the three crystallographically distinct octahedral sites: M1, M2, and M3. At low pressures we find, as expected, that iron in wadsleyite adopts its high spin state. The enthalpy differences from our high-spin calculations are consistent with the experimental observations that the M2 site is depleted in iron and independent of the magnetic moment of iron. This finding indicates that the inter-octahedral site partitioning of iron is due to the presence of the d-orbitals. If this finding can be corroborated our results will affect the understanding of the partitioning of other divalent transition metals and geochemical trace elements in wadsleyite, the most abundant mineral in the upper part of the Earth's transition zone.

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