

Abstract Submitted
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α - to β - to γ -spinel transformations in Mg_2SiO_4 .¹ ZHONGQING WU, YONGGANG YU, RENATA WENTZCOVITCH, Minnesota Supercomputing Institute and Department of Chemical Engineering and Materials Science, University of Minnesota, 421 Washington Ave SE — Phase relations in Mg_2SiO_4 have been investigated by first principles quasiharmonic calculations. The α - to β -spinel transition is believed to cause the 410-km discontinuity, while the β - to γ -spinel transformation may contribute to the 520-km discontinuity. We have obtained these phase boundaries using LDA and PBE/GGA exchange correlation functionals and results confirm the trend usually displayed by these functionals. Information on this series of transformations in Mg_2SiO_4 will help us understand the importance of other elements on this sequence of phase transformations across the Earth's transition zone.

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