



Spin crossover in ferropicrlase from first-principles molecular dynamics simulations

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Ferropicrlase is the second-most abundant mineral of the lower mantle of the Earth. It is experimentally known that with increasing pressure, the iron ions in the mineral begin to collapse from a high-spin to low-spin state. This spin crossover alters various properties of the material, and hence a good theoretical understanding of the phenomenon is necessary. Using first-principles molecular dynamics simulations in conjunction with thermodynamic integration, we construct a phase diagram of the spin crossover as a function of pressure and temperature. In addition, we present the thermal equation of state of the mineral up to 140 GPa and 4000 K, and predict that the electrical conductivity of ferropicrlase reaches semi-metallic values within the lower mantle.