Abstract Submitted
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Crystalline-gel-molten phase transitions of water in calcium dipicolinate (Ca-DPA)[1] SUBODH TIWARI, ANKIT MISHRA, CHUNYANG SHENG, PANKAJ RAJAK, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — The heat resistance of bacterial spores directly correlates to the protoplast dehydration and presence of dipicolinic acid (DPA) and its associated metal salts at the core. Bacteria's structural integrity in moist heat conferred by high concentration of DPA and calcium DPA salts depends on the properties are additional water molecules and temperature. In our reactive MD simulations, we characterize different possible phases and the transport properties of water molecules. We observed solid-gel and gel-liquid phase transitions of the hydrated Ca-DPA system. These simulations reveal monotonically decreasing solid-gel-liquid transition temperatures with increasing cell hydration, reflecting the experimental trend of moist-heat resistance of bacterial spores. We also observed that the calcification of bacterial spores further increases the transition temperatures.

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