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Dissolved carbon in extreme conditions characterized by first principles simulations[1] DING PAN, GIULIA GALLI, Institute for Molecular Engineering, the University of Chicago — One key component to understanding carbon transport in the Earth interior is the determination of the molecular species formed when carbon bearing materials are dissolved in water at extreme conditions. We used first principles molecular dynamics to investigate oxidized carbon in water at high pressure (P) and high temperature (T), up to the conditions of the Earth's upper mantle. Contrary to popular geochemistry models assuming that CO_2 is the major carbon species present in water, we found that most of the dissolved carbon at 10 GPa and 1000 K is in the form of solvated CO_3^{2-} and HCO_3^- anions. We also found that ion pairing between alkali metal cations and CO_3^{2-} or HCO_3^- anions is greatly affected by P-T conditions, decreasing with pressure along an isotherm. Our study shows that it is crucial to take into account the specific molecular structure of water under extreme conditions and the changes in hydrogen bonding occurring at high P and T, in order to predict chemical reactions in dissolved carbon. Our findings also shed light on possible reduction mechanisms of CO_2 when it is geologically stored, depending on the availability of water.

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