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Supplementary Materials for

The fate of carbon dioxide in water-rich fluids under extreme conditions

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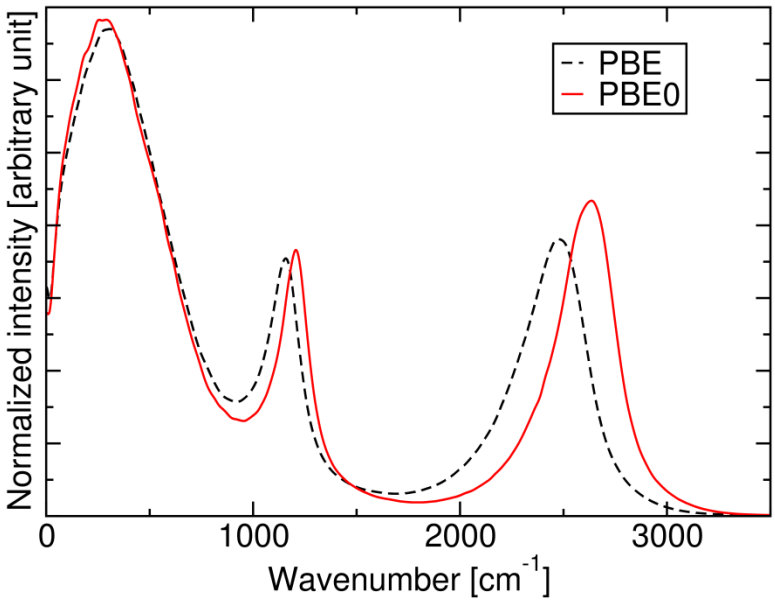

fig. S1. The vibrational density of states of the 0.9 *m* Na_2CO_3 solution at ~11 GPa and 1000 K. Two exchange-correlation functionals, PBE and PBE0, are compared.

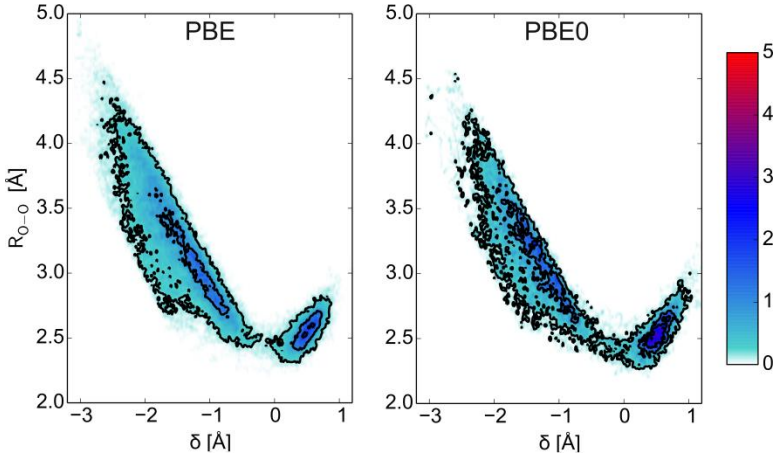

fig. S2. Probability distributions of positions of protons hopping between CO_3^{2-} and H_2O in the Na_2CO_3 solution at 0.2 GPa and 823 K. The unit is $Å^{-2}$. The reaction coordinate $R_{O\text{-}O}$ is the distance between the two neighboring oxygen atoms, O_c and O_w, in carbonate ions and water molecules respectively, and δ is the proton displacement $R_{Oc\text{-}H}$ -$R_{H\text{-}Ow}$. Two xc functionals were compared: PBE and PBE0.