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The dissociation constant of water at extreme conditions OTTO E. GONZALEZ-VAZQUEZ, International Center for Theoretical Physics "Abdus Salam" (ICTP), LUIGI GIACOMAZZI, International Center for Theoretical Physics "Abdus Salam" (ICTP), The International School for Advanced Studies (SISSA), C. PINILLA, SANDRO SCANDOLO, International Center for Theoretical Physics "Abdus Salam" (ICTP) — Only one out of 10^7 water molecules is dissociated in liquid water at ambient conditions, but the concentration of dissociated molecules increases with pressure ad temperature, and water eventually reaches a fully dissociated state when pressure exceeds 50-100 GPa and temperature reaches a few thousand Kelvin. The behavior of the dissociation constant of water (pKa) at conditions intermediate between ambient and the fully dissociated state is poorly known. Yet, the water pKa is a parameter of primary importance in the aqueous geochemistry as it controls the solubility of ions in geological fluids. We present results of molecular dynamics calculations of the pKa water at extreme conditions. Free-energy differences between the undissociated and the dissociated state are calculated by thermodynamic integration along the dissociation path. The calculations are based on a recently developed all-atom polarizable force-field for water, parametrized on density-functional theory calculations.

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