

# **Effects of Thermodynamic Ensemble and Mineral Surface on Interfacial Water Structure**

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Supplementary Material

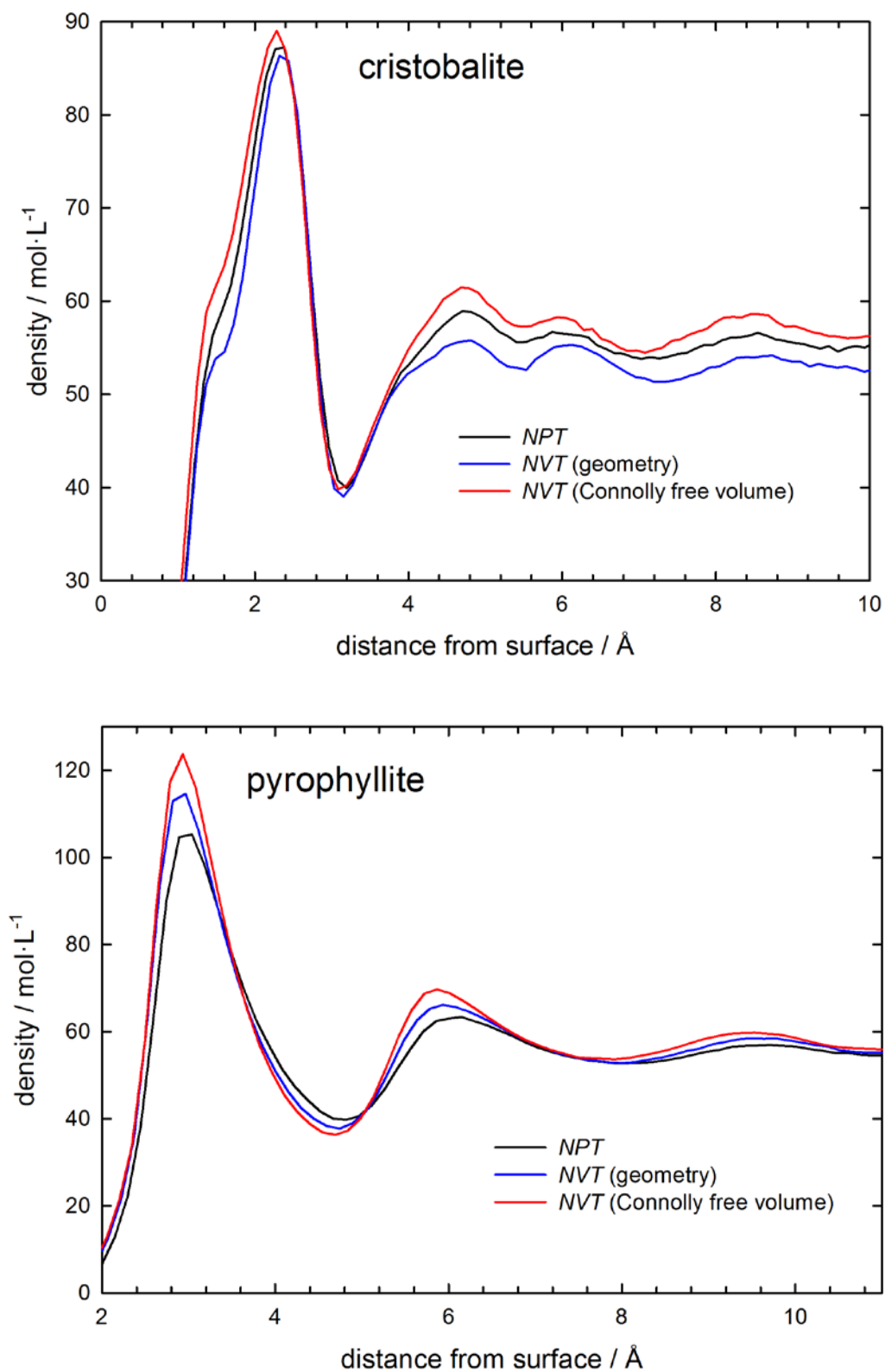


Figure S1. Water oxygen density profiles near the surface of cristobalite (111) (top) and pyrophyllite (001) (bottom) based on  $10^5$  configurations over 10 ns.

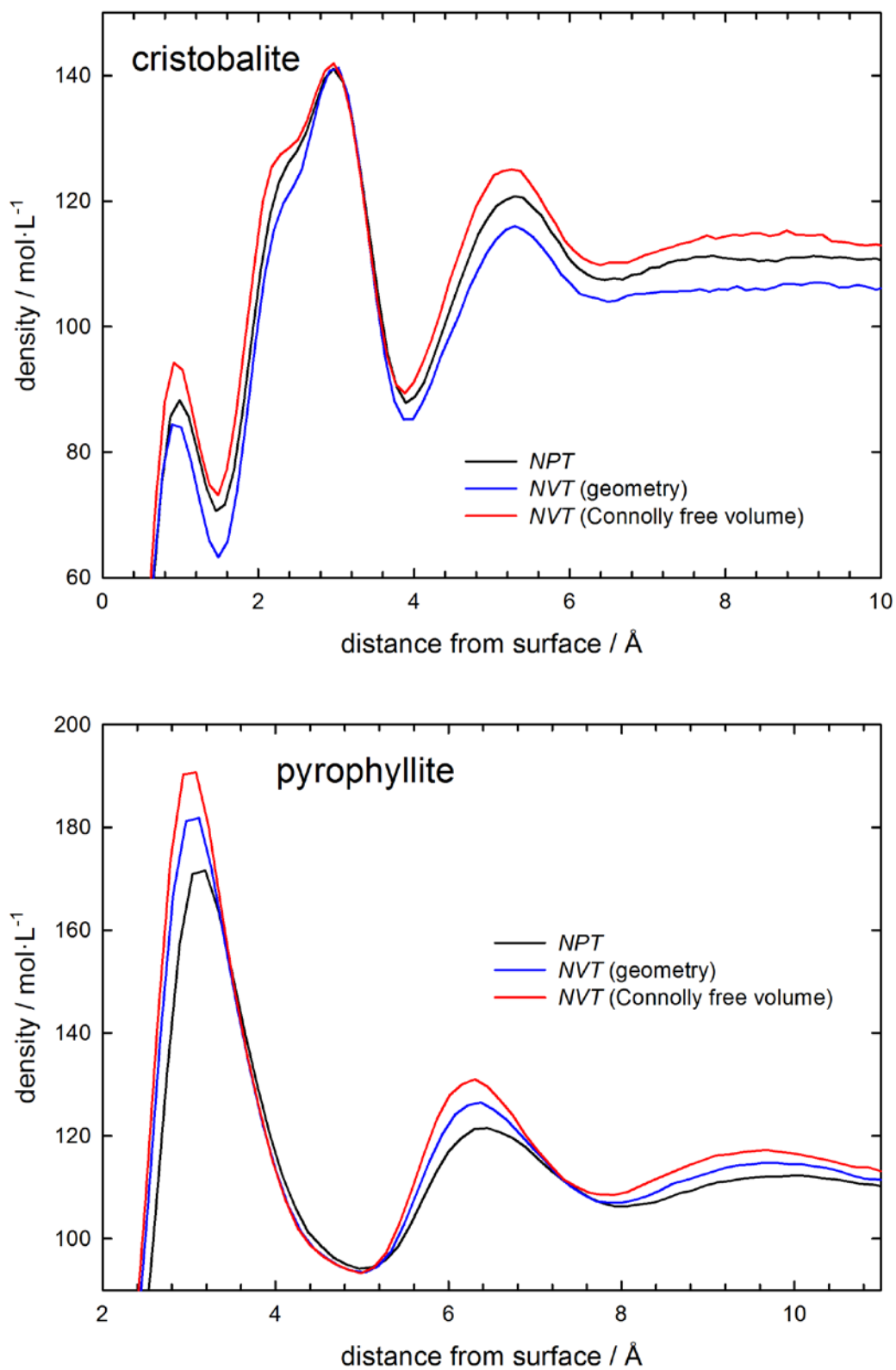


Figure S2. Water hydrogen density profiles near the surface of cristobalite (111) (top) and pyrophyllite (001) (bottom) based on 10<sup>5</sup> configurations over 10 ns.