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Ab initio molecular dynamics simulations using a Chebyshev-filtered subspace iteration technique for modeling amorphous silicon dioxide[1] MINJUNG KIM, KHOONGHONG KHOO, JAMES CHELIKOWSKY, University of Texas — Ab initio molecular dynamics simulations are a powerful tool for examining liquids and amorphous materials; however, such simulations are often computationally intensive. We present a molecular dynamics method that dramatically reduces the computational load using a new algorithm based on Chebyshev-filtered subspace iteration. We apply this method to amorphous silicon dioxide. Amorphous silicon dioxide has been intensively studied owing to its broad applications to electronic devices and photonics. We perform ab initio molecular dynamics simulations to obtain the amorphous structure of silicon dioxide. We employ implement several new procedures to investigate the effect of quenching rates and system sizes. The calculated structure factor for our amorphous structure is in good agreement with experimental data. We performed structural relaxations to calculate the hyperfine splitting constants. Our calculated hyperfine splitting constants of E'_γ oxygen defect centers show excellent agreement with electron paramagnetic resonance experiments. We will also discuss statistical results of oxygen-related defect centers.

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