Ab initio molecular dynamics investigation of SiO_2 precipitation in Earth's core

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Silicon and oxygen have attracted considerable attention as potential light elements in Earth's core, because their stronger affinity to metal observed in high pressure experiments with increasing temperature in core-forming conditions suggests a significant amount of both could be incorporated into the core. It was recently proposed that SiO_2 could crystallize from a ternary Fe-Si-O liquid alloy at the top of the core during secular cooling, leaving the present-day core with either silicon or oxygen, but not both. We investigated the liquidus field of the Fe-Si-O ternary using ab initio molecular dynamics at core-mantle boundary pressure (136 GPa) and a range of temperatures (3800 K to 4800 K), encompassing any plausible value for the core through geologic time. Using four independent lines of argumentation, we find no evidence for SiO_2 crystallization, or even phase separation. Furthermore, simulations on Fe-Si and Fe-O binaries and their comparison with Fe-Si-O ternaries show that iron, silicon, and oxygen mix ideally at core conditions, confirming that ternary equations of state can reliably be obtained from ideal mixing of binary properties.