# First-principles simulations of SiO2 melt: Compression behavior and melting properties at the lower mantle pressure conditions

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Silica is an exclusively important material in various fields including material science, solid state physics, and Earth science, because it is a most major component of glasses and magmas. It is known that at low pressures, $SiO_2$ melt is composed of $SiO_4$ tetrahedra, which shows interesting properties such as density inversion and liquid-liquid phase transition at about 5 GPa. Clarifying the physical properties of $SiO_2$ melt under pressure might be a key to understand the thermal, chemical, and dynamical properties of the Earth's interior, in particular the seismic ultra-low velocity zone (ULVZ) which has been detected locally at the core-mantle boundary (CMB). However, study on the melting properties of $SiO_2$ at the lower mantle pressures is very limited. Although classical molecular dynamics simulations determined pressure evolution of its liquidus [Belonoshko and Dubrovinsky, 1995], reliability of the empirical force fields applied is highly unclear. Here, we perform first-principles molecular dynamics (FPMD) simulations of $SiO_2$ melt to investigate its structural and melting properties at ultra-high pressures. Our melting curve of $SiO_2$ shows a significant difference from the result of Belonoshko and Dubrovinsky (1995). Research supported by JSPS and Ehime Univ Project Fund.