# Modeling silicate melt

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Silicate melt is a complex network liquid composed of $SiO_n$ (n=4-6) polyhedra with other elements such as silicon, oxygen, aluminum, alkalis, magnesium, iron *etc*. Knowing its physical properties is of great importance in understanding geophysical processes in history of Earth, Moon and other terrestrial planets. Therefore its physical properties at low pressure have been theoretically studied with some success by using molecular dynamics simulation with empirical force fields. However, empirical force fields often fail to describe the behavior of silicate melts at high pressure, where only few experimental data are available for fitting potential parameters. First principle molecular dynamics simulation is expected to play an important role in studying silicate melts, such as magma ocean[1], in a wide range of temperature and pressure condition.

It is well known that diffusivity and viscosity of silicate melts calculated with empirical force fields much more strongly depend on the size of the simulation cell than those of liquid water[2-4]. Only model silicate melt with simple stoichiometry in a small simulation cell can be investigated with first principles simulation due to its huge computational cost. Then questions arise: How large simulation cell and how long simulation time are needed for the convergent results of the transport properties? How is it possible to extrapolate the results for a small cell to obtain the results for an infinite cell? What is the physics behind the size dependence? How large simulation cell and how long simulation time can be achieved with conventional and order-N first principles simulations? How can we construct empirical force fields from first principle simulation data? I will discuss these questions.

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