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First-principles simulations of grain boundaries and crystal-melt interfaces in Mg_2SiO_4 under pressure

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Grain boundaries and crystal-melt interfaces play vital role in various geophysical and geochemical processes of Earth's interior. However, the knowledge of these interfaces in key mantle minerals at relevant pressures is still limited. Here we present the results of our large-scale first-principles molecular dynamics simulations on the structures and energetics of grain boundaries and crystal-melt interfaces in Mg_2SiO_4 in the pressure range 0 – 20 GPa at 0 and 1500 K. For solid-solid (grain boundary) interfaces, the calculated formation enthalpy gradually increases with pressure lying in the range 0.8 – 1.6 J/m^2, being consistent with experimentally inferred values. Our results show that the solid-liquid interfacial enthalpy is larger than the grain boundary enthalpy at low pressure and the two enthalpies become comparable as pressure increases. The addition of hydrous component (H_2O) tends to lower the formation enthalpy of these interfaces. For instance, the formation enthalpy of some hydrous grain boundaries lies below 1.0 J/m^2 over the entire pressure regime considered. The calculated enthalpy results are further used to estimate dihedral angle, which is relevant to understand grain-scale distribution of partial water-bearing melts in the upper mantle.