Ma-003 Room: C403 Time: June 26 10:00-10:15

Molecular dynamics simulation of the NaAlSiO4 high pressure phase with the CaFe2O4 structure

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The possible existence of the high pressure NaAlSiO4 phase with the CaFe2O4 structure has previously been proposed. We have applied MD simulation to investigate its crystal structure, energetic stability, and compressibility.