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First principles study on the phase stability and elasticity of potassium-host hexagonal aluminous phases

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In order to understand the fate of the potassium-bearing phase subducted into the deep Earth's interior, we have studied the high-pressure stability and elasticity of KMg2Al5SiO12 hexagonal aluminous phase (K-Hex) by means of the density functional computation method. The K-Hex phase is found to be mechanically stable up to 150 GPa and also energetically more stable than the calcium-ferrite (K-CF) type structure up to 150 GPa. In addition, calculations indicate that when the spinel composition coexists with the K-hollandite (K-Hol) phase, the K-Hex phase becomes more stable than the K-Hol phase at pressures above ~27 GPa. This suggests that the hexagonal aluminous phase be a potential host of the incompatible large-ion elements such as potassium in the lower mantle, especially in the subducted basaltic Mg and Al rich composition. Finally, seismic velocities of the K-Hex phase are found slower than Mg-perovskite (pv) in the lower mantle pressures, while its density is larger than Mg-pv over 70 GPa.

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