Ab initio calculations of elastic constants of plagioclase feldspars

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ABSTRACT

Plagioclase feldspars comprise a large portion of the Earth's crust and are very anisotropic, making accurate knowledge of their elastic properties important for understanding the crust's anisotropic seismic signature. However, except for albite, existing elastic constants for plagioclase feldspars are derived from measurements that cannot resolve the triclinic symmetry. We calculate elastic constants for plagioclase end-members albite $NaAlSi_3O_8$ and anorthite $CaAl_2Si_2O_8$ and intermediate andesine/labradorite $NaCaAl_3Si_5O_{16}$ using density functional theory to compare with and improve existing elastic constants and to study trends in elasticity with changing composition. We obtain elastic constants similar to measured elastic constants and find that anisotropy decreases with anorthite content.

Keywords: Plagioclase feldspars, elastic constants, ab initio calculations, seismic anisotropy