Ab initio calculations of elastic constants of plagioclase feldspars PAMELA KAERCHER^{1,*}, BURKHARD MILITZER^{1,2} AND HANS-RUDOLF WENK¹

¹Department of Earth and Planetary Science, University of California, Berkeley, California 94720, U.S.A. ²Department of Astronomy, University of California, Berkeley, California 94720, U.S.A.

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 NaAlSi₃O₈ and anorthite CaAl₂Si₂O₈ and intermediate andesine/labradorite NaCaAl₃Si₅O₁₆ 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