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First-principles calculation of the elastic moduli of sheet silicates and their application to shale anisotropy

B. Militzer,[1,2,*] H.-R. Wenk,[1] S. Stackhouse,[1] and L. Stixrude[3]

[1]Department of Earth and Planetary Science, University of California, Berkeley, California 94720, U.S.A.
[2]Department of Astronomy, University of California, Berkeley, California 94720, U.S.A.
[3]Department of Earth Sciences, University College London, Gower Street, London WC1E 6BT, U.K.

Abstract

The full elastic tensors of the sheet silicates muscovite, illite-smectite, kaolinite, dickite, and nacrite have been derived with first-principles calculations based on density functional theory. For muscovite, there is excellent agreement between calculated properties and experimental results. The influence of cation disorder was investigated and found to be minimal. On the other hand, stacking disorder is found to be of some relevance for kaolin minerals. The corresponding single-crystal seismic wave velocities were also derived for each phase. These revealed that kaolin minerals exhibit a distinct type of seismic anisotropy, which we relate to hydrogen bonding. The elastic properties of a shale aggregate was predicted by averaging the calculated properties of the contributing mineral phases over their orientation distributions. Calculated elastic properties display higher stiffness and lower p-wave anisotropy. The difference is likely due to the presence of oriented flattened pores in natural samples that are not taken into account in the averaging.

Keywords: Elasticity, clay, ab initio calculations, sheet silicates, seismic anisotropy