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First-principles studies on the elastic constants of a 1:1 layered kaolinite mineral

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ABSTRACT

The mechanical behavior of minerals under high pressure has attracted considerable interest in recent years. Clay minerals, including kaolinite, are common minerals found in sedimentary environments and their behavior under pressure is an important factor in understanding seismogenic zones. Kaolinite is a ubiquitous member of the kaolin group of 1:1 phyllosilicates that have recently been found to undergo a structural phase transition between 2.0 and 2.5 GPa. In this study, the bulk modulus and elastic constants of kaolinite have been calculated from first principles within density functional theory (DFT) for the first time. The bulk modulus is predicted to be 23 GPa for kaolinite. The calculated elastic constant tensors indicate that the **a** direction is slightly more flexible than the **b** direction. The calculated elastic constant tensor along **c** is much lower than the constants calculated along **a** and **b** consistent with the crystal structure of kaolinite. Elastic wave velocities for P- and S-waves were calculated to be 7.34 and 3.50 km/s, respectively. Since an agreement between the theoretical and experimental values is satisfactory, we conclude that the theoretical calculations presented here are useful in seismic research for predicting the mechanical properties of minerals that are difficult to obtain experimentally because of their small particle size (typically <2 micrometers).