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First-principles modeling of the infrared spectrum of kaolinite

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ABSTRACT

The theoretical infrared spectrum of kaolinite [$Al_2Si_2O_5(OH)_4$, triclinic] was computed using ab initio quantum mechanical calculations. Calculations were performed using the Density Functional Theory and the generalized gradient approximation. The low-frequency dielectric tensor of kaolinite was determined as a function of the light frequency using linear response theory. The IR spectrum was then calculated using a model that takes into account the shape and size of kaolinite particles. A remarkable agreement was obtained between theory and experiment, especially on the position of the stretching bands of OH groups. This agreement provides a firm basis for the interpretation of the IR spectrum of kaolinite in terms of structural parameters.