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First-principles study of OH-stretching modes in kaolinite, dickite, and nacrite

ETIENNE BALAN,[1,2,*] MICHELE LAZZERI,[1] A. MARCO SAITTA,[3] THIERRY ALLARD,[1] YVES FUCHS,[4]
AND FRANCESCO MAURI[1]

[1]Laboratoire de Minéralogie-Cristallographie, UMR CNRS 7590, Universités Paris VI et VII, IPGP, 4 Place Jussieu, 75252 Paris Cedex 05, France
[2]UR 058 GEOTROPE, Institut de Recherche pour le Développement (IRD), 213 rue La Fayette, 75480 Paris Cedex 10, France
[3]Laboratoire de Physique des Milieux Condensés, UMR CNRS 7602, Université Paris VI, 4 Place Jussieu, 75252 Paris Cedex 05, France
[4] Laboratoire des Géomatériaux, IFI, Université de Marne La Vallée, FRE CNRS 2455, 5 Allée Descartes, 77454 Champs sur Marne, France

ABSTRACT

The OH-stretching modes of kaolinite group minerals, namely kaolinite, dickite, and nacrite, are investigated within the density functional theory framework. Good agreement between theoretical and experimentally derived structures is obtained. The total energy of the three polymorphs is found to be similar within 1 kJ/mol. After a review of existing experimental data, infrared and Raman spectra of the three polymorphs are computed. While interpreting the spectra, special attention is given to the role played by the macroscopic geometry of the system, explaining the differences experimentally observed between infrared and Raman spectra. In dickite and nacrite, a significant interlayer coupling is observed for the modes polarized along a direction nearly parallel to **c***. The assignment of OH-stretching bands is given in a consistent way and is compared with previous suggestions.