

## **A lattice dynamical study of the aragonite and post-aragonite phases of calcium carbonate rock**

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### **ABSTRACT**

A recent force field model is used in this paper to analyze, with a nano-scale simulation, the structural and the vibrational properties of a rock system under the application of various high pressures. Our results show that this model reproduces accurately the equilibrium structural properties for calcite, gives comparable results for aragonite with the observed data, and predicts the structural, elastic and vibrational properties of the post-aragonite phase.

In addition, we show that the transition from the aragonite to the post-aragonite phase appears at a transition pressure of 35.2 GPa. The longitudinal wave velocity increases rapidly by a factor of 1.71. In contrast the shear wave velocity increases very slowly up to the transition pressure, and thereafter increases rapidly, changing by 45% to 80 GPa. In addition, our calculations for the vibrational properties show that with the new potential model presented here, we observe a softening mode in the  $\Gamma$ -F direction. The phonon frequencies of the post-aragonite phase show more modes than for calcite and aragonite.

**Keywords:** Molecular dynamics, calcite rock, lattice dynamic