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High-Pressure Phase Transition in Some Alkali Halides Using Interatomic Potential Model

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<u>Abstract:</u> We have predicted the phase transition pressure in some alkali halides NaCl and KCl using an interatomic potential approach based on a rigid ion model. We have obtained phase transition pressures 28.69 and 2.4 GPa, respectively, and are in close agreement with their corresponding experimental transition pressures 29.0 and 2.0 GPa. This approach is promising with respect to the prediction of the phase transition pressures of other alkali halides.

Key Words: Alkali halide, phase transition, interatomic potential



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