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STUDY OF PHONON DENSITY OF STATES IN GRAPHITE USING DENSITY FUNCTIONAL THEORY

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This study computes the phonon density of states (PhDOS) of graphite using first-principles density functional theory (DFT) with the open-source Quantum ESPRESSO package. The results provide insights into the vibrational properties of crystalline graphite that govern thermal scattering processes. The phonon spectrum, regarded as a probability density function, serves as essential input for further investigations of the thermal neutron scattering law S(α, β) and neutron cross-section evaluations. Incorporating phonon effects into neutron interaction models is expected to enhance the accuracy of thermal neutron cross-section calculations. These preliminary results represent a step toward the systematic evaluation of thermal neutron cross-sections for crystalline materials.
Keywords: Graphite; first-principles study; phonon density of state (PhDOS); thermal neutron cross-section.

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