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PhDAssistance provides D3Q expert where you can hire expert trained to perform molecular dynamics i.e., simulate the density functional perturbation theory for systems with hundreds to millions of particles.

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- · Derivative of total energy from three phonons from density functional perturbation theory
- · Three-body force constants
- · Phonon-phonon interaction from anharmonici ty, isotopes and boundary scattering
- Phonon line width/lifetime and 3rd order line shift

- · Phonon spectral function
- Thermal conductivity in the single-mode approx imation
- · Thermal conductivity from iterative diagonaliza tion of the linearized Boltzmann equation
- Final state decomposition of phonon decay •
- · Quasi harmonic approximation

– More

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