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Influence of Hamiltonian on the properties of NaCl[1] RYAN JACOB, A.R. CHOURASIA, Department of Physics, Texas A&M University-Commerce — Sodium chloride has been investigated using the CRYSTAL98 code to determine its properties. The geometry and the basis set have been optimized prior to analysis. The analysis was carried out using the different Hamiltonians: Restricted Hartree-Fock, Unrestricted Hartree-Fock, Restricted open shell Hartree-Fock, and the DFT. In the DFT the B3PW and B3LYP potentials have been used. The physical properties have been calculated and compared with the experimental values. The present investigation is aimed at studying the usefulness and limitations of the code.

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