

Molecular solids are important materials with many applications in various fields of science and industry. They are often characterized by a rich phase diagram and the ability to adopt multiple crystal structures (polymorphism). To describe small energy differences between various phases or polymorphs, accurate quantum mechanical methods are needed. In this thesis, lattice energies of methane, methanol, ammonia, and carbon dioxide are calculated using two different approaches, namely, the fragment approach and the periodic boundary conditions (PBC) approach. These two schemes have different requirements in terms of compute cost and human time needed to obtain precise results. In the fragment scheme, the Hartree-Fock, MP2, and CCSD(T) quantum mechanical methods are employed. In the PBC scheme, the Hartree-Fock and MP2 lattice energies are calculated. For all four systems, which differ in the nature of prevalent intermolecular interactions, a very good agreement in the range of 0.1 – 0.6 kJ/mol was found between both approaches at the MP2 level.