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Elastic properties and phase stability of AgCl under external pressure[1] ALEJANDRO BAUTISTA-HERNÁNDEZ, PEDRO H. HERNÁNDEZ, GREGORIO HERNÁNDEZ-COCOLETZI, J. FRANCISCO RIVAS-SILVA, Universidad Autónoma de Puebla — Ab initio total energy calculations have been performed to study AgCl phase stabilities. Our calculations are done using the density functional theory within the local density approximation, for the exchange and correlation energies. The ion-electron interactions are treated with the Troullier-Martins pseudopotentials. We determine the equation of state and free energy in the B1 (NaCl) and B2 (CsCl) phases. To obtain the elastic constants, we take the second derivative of the total energy respect to the applied deformations in both B1 and B2 phases. Our calculated structural parameters of the phases B1 and B2 of AgCl are compared with those available experimental data and theoretical calculations based on the local density approximation. The stability analysis based on elastic coefficients yields a critical pressure of 6 GPa at which the ideal lattice of B1 structure becomes unstable against homogeneous tetragonal shear deformation. The B2 structure is unstable in the interval of pressures 0-25 GPa. Therefore, a pressure induced phase transition between the structures B1 and B2 is not allowed elastically. We also explore the atomic structure of AgCl in the KOH phase.

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