Study of structural and thermal properties of SiO2 and Al2O3 in the Diatomite

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Abstract : Diatomite is a light colored rock formed entirely or substantially of "backbones" of diatoms. These unicellular algae are surrounded by a "shell" in silica, frustule, the accumulation of the substance can lead to the formation of a rock.In this work we determine the structural and thermal properties of SiO2 and Al2O3 in the diatomite using the plane wave method and linearized augmented (LAPW) in the functional theory of density (DFT).The potential for exchange and correlation is calculated by the generalized gradient approximation (GGA).Regarding thermal properties, we calculated the free enthalpy G, S entropy, specific heat C, thermal conductivity ? ..... etc of SiO2 and Al2O3 component. The temperatures used in this work are 1400, 1450 and 1500 respectively;The results are in good agreement with some experimental data.

Keywords : DFT1, diatomite, thermal proprieties