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Investigating the Molecular Behavior of H_2O in Caso 4 -2h₂o Two-Dimensional Nanoscale System

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Abstract : A molecular fluids' behavior and interaction with other materials at the nanoscale is a complex process. Nanoscale fluids behave so differently than macroscale fluids and interact with other materials in unique ways. It is, therefore, feasible to understand the molecular behavior of H_2O in such two-dimensional nanoscale systems by studying (CaSO4-2H2O), commonly known as gypsum. In the present study, spectroscopic measurements on a 2D structure of exfoliated gypsum crystals are carried out by Raman and IR spectroscopy. An array of gypsum flakes with thicknesses ranging from 8nm to 100nm were observed and analyzed for their Raman and IR spectrum. Water molecules stretching modes spectra lines were also measured and observed in nanoscale gypsum flakes and compared with those of bulk crystals. CaSO4-2H2O crystals have Raman and infrared bands at 3341 cm-1 resulting from the weak hydrogen bonds between the water molecules. This internal vibration of water molecules, together with external vibrations with other atoms, are responsible for these bands. There is a shift of about 70 cm-1 In the peak position of thin flakes with respect to the bulk crystal, which is a result of the different atomic arrangement from bulk to thin flake on the nano scale. An additional peak was observed in Raman spectra around 2910-3137 cm^{-1} in thin flakes but is missing in bulk crystal. This additional peak is attributed to a combined mode of water internal (stretching mode at 3394cm^{-1}) and external vibrations. In addition to Raman and infra- red analysis of gypsum 2D structure, electrical measurements were conducted to reveal the water molecules transport behavior in such systems. Electrical capacitance of the fabricated device is measured and found to be (0.0686 *10-12) F, and the calculated dielectric constant (ε) is (12.26).

Keywords : gypsum, infra-red spectroscopy, raman spectroscopy, H_2O behavior
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