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CO_2 and CH_4 clathrate hydrate under pressure J.M. MENÉNDEZ, Departamento de Química Física y Analítica, Universidad de Oviedo, Oviedo, Spain, A. OTERO-DE-LA-ROZA, School of Natural Sciences, University of California, Merced, USA, F. IZQUIERDO, V. MUÑOZ, L. JIMENEZ, O. PRIETO-BALLESTEROS, Centro de Astrobiología (INTA-CSIC), Madrid, Spain, J.M. RECIO, Departamento de Química Física y Analítica, Universidad de Oviedo, Oviedo, Spain, MALTA CONSOLIDER TEAM — DFT first principles calculations have been performed to study the response to hydrostatic pressure of sI-type CO2 and CH4 clathrate hydrates. Two kinds of simulations were carried out i) periodic crystalline structures were considered to optimize unit cell geometries, determine static equation of state parameters, and investigate the energetic stability of clathrates. Dispersion interactions have been accounted for by the exchange-hole dipole moment model recently implemented for solid state calculations. It is found that, gas filling is a stabilization process independent on the guest molecule. However, while CH4 shows no preference for the size of the cage, the effect of stabilization is more pronounced when CO2 is in $5^{12}6^2$ cages. Pressure also favors stabilization of both molecules, with CO2 being more sensitive than methane. ii) Molecular calculations using finite clusters were also carried out. At selected geometries, vibrational frequencies and intensities have been computed for all the gas-cage combinations. A change in the vibrational modes due to the confinement of the guest molecules is revealed. However, pressure barely affects the Raman/IR spectrum of the clathrate. These theoretical findings will be compared with experimental data already in progress

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