Energetics of Highly Porous Solids

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Highly porous solids, including zeolites, mesoporous silicas, and metal organic frameworks (MOF) are important as catalysts and ion exchangers. Systematic experimental calorimetric studies of their thermochemical properties have revealed a number of systematic trends. Firstly, despite increases in molar volume of factor of 2 to 10 relative to dense phases, these porous frameworks are only modestly destabilized in energy by 10 - 30 kJ per mole. Different structures form a dense energy landscape, enabling the synthesis of many new polymorphs. These frameworks contain guest molecules: H2O, CO2, and organics.. The energy of host-guest interactions has been studied by gas adsorption microcalorimetry which enables the measurement of interaction energy versus coverage , resulting in a complex picture of several microscopic steps of adsorption. Such interactions are weak when specific bonds are not formed bugt can be quite strong if direct bonding to a metal center occurs. SXeveral detailed examples will be presented.