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Storage capacity of clathrate hydrates for storing small molecules

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Density functional theory (DFT) based studies are carried out to understand the structure, stability and reactivity of clathrate hydrates with or without hydrogen encapsulation. All geometries of clathrate hydrates were fully optimized using B3LYP/6-31G(d), M06-2X/6-31G(d) and B97D/6-31G(d) level of theories. The storage capability of five standard clathrate hydrates (5^{12} , $4^35^66^3$, $5^{12}6^2$, $5^{12}6^4$ and $5^{12}6^8$) is systematically explored to store small molecules like Ar, CH_4 , CO_2 , H_2 , H_2S , Kr, N_2 , O_2 and Xe. The capability is depicted in the given Figure. The efficacy of trapping of small molecules inside the cages of clathrate hydrates generally depends upon the cavity sizes and shapes. The interaction energy values indicate the formation of stable guest-host system.

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