OH-IRMOF-16 as potential drug carrier for Gemcitabine delivery. A DFT study.

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The unique physical and chemical characteristics of Metal Organic Frameworks (MOFs) make them promising candidates for drug storage and drug delivery. MOFs are organic – inorganic hybrid materials made of metal ions or clusters interconnected through an organic linker. In order to develop new and much-improved drug delivery regimes in IRMOF-16 we functionalized each organic linker with a hydroxyl group. Then, the interaction of gemcitabine with the strategically modified organic linker of IRMOF-16 (non-toxic, high-loading MOF) has been investigated by employing DFT methods (PBE/TZVP). Our results indicate that the introduction of a hydroxyl group in the organic linker of IRMOF-16 was critical for gaining key acid-base and hydrogen-bond interaction sites. The maximum interaction energy with gemcitabine was found to be 24 kcal/mol for the modified IRMOF-16. Semi-empirical calculations (PM7) were also performed in order to study the interactions of gemcitabine with larger fragments of the modified IRMOF-16 unit cell.