

# Precise Regulation of Active Sites of MOFs for Capture of Iodine

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## Abstract

Metal-organic frameworks (MOFs) have great potential for the capture of volatile iodine. The effect of a precise regulation of active sites in JLNU-4 (MOFs) on capture of iodine was investigated by Monte Carlo (MC) method and molecular dynamics (MD), and it was found that the larger the Zn/Cd atomic ratio, the better the iodine capture. Interestingly, compared with the meta-position regulation of Zn/Cd, the ortho-positions regulation increased the free volume of the crystal and enhanced the interaction between Cd and I, thus improving the capture capacity of iodine. The first-principles study revealed the charge transfer of each atom in the MOFs crystal with I<sub>2</sub> during iodine capture and the secondary bonds with weak covalent interactions were all formed after I<sub>2</sub> adsorption onto MOFs. These findings provide a reference for the capture of radioactive iodine and a theoretical basis for the strategies for precise regulation of MOFs in the future.

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