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Molecular Simulations for Adsorptive Separation of CO_2/CH_4 Mixture in Metal-Exposed, Catenated, and Charged Metal−Organic Frameworks

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This article was the highlighted cover article for *Langmuir* Volume 25, Issue 9. Due to a production error, the wrong text for the On the Cover statement, which appears at the end of the Table of Contents, was published in the print version of the issue. The Web version contains the correct On the Cover statement. The correct statement is as follows:

On the Cover: Cover illustration by Ravichandar Babarao and Jianwen Jiang. Natural gas is an ideal substitute for environmentally unfriendly fossil fuels. To increase the calorie content of natural gas, it is crucial to remove impurities such as CO_2. In this work, molecular simulations are carried out for the adsorptive separation of a CO_2/CH_4 mixture in a series of MOFs with unique characteristics including exposed metals (Cu-BTC, PCN-6′, and PCN-6), catenation (IRMOF-13 and PCN-6) and extraframework ions (soc-MOF). The exposed metals and catenation are found to slightly enhance the selectivity of CO_2 over CH_4. The extraframework ions NO_3^- in charged soc-MOF act as additional adsorption sites for quadrupolar CO_2 molecules, and the selectivity in soc-MOF is 1 order of magnitude higher than in IRMOFs and PCNs and the highest among various MOFs reported to date. [CO_2, dumbbell balls and sticks; CH_4, green balls; framework, CPK model]. For more information, see "Molecular Simulations for Adsorptive Separation of CO_2/CH_4 Mixture in Metal-Exposed, Catenated, and Charged Metal−Organic Frameworks" by Ravichandar Babarao, Jianwen Jiang, and Stanley I. Sandler on pages 5239−5247 of this issue.