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Simulations of adsorption of CO2 and CH4 in MOFs: effect of the size and charge distribution on the selectivity SIDI MAIGA, SILVINA GATICA, Department of Physics, Howard University — Using the method of Grand Canonical Monte Carlo we have computed the adsorption of CO2 and CH4 in MOFs with a periodic cubic structure. We used a model of the MOF that allows systematic variations in the charge distribution, size and LJ parameters. We estimated the selectivity of CO2 over CH4 for different temperatures in MOFs with various sizes and charge distributions. The results show that inserting dipoles at the corners of the MOF's unit cell would increase the selectivity of CO2; on the other hand adding quadrupoles to the structure is ineffective. The size of the cell strongly affects the adsorption of CO2 and selectivity: compressing the cell in only 10% significantly increases the selectivity; expanding the cell by 20% reduces it. Regarding thermal effects, we estimated that the selectivity drops from 250 to 2 when the temperature rises from 140K to 300K. Although this model is inspired by the IRMOF-1, which has a cubic unit cell, it can be adapted to represent other MOFs with noncubic structures by modifying the geometry accordingly. This work implies that MOFs suit gas separation.

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