Induced Selective N_2 Binding under Electric Field: Application for the Separation of N_2/CH_4 and N_2/CO_2

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Dinitrogen is the most abundant species in the air and an inert gas molecule which makes it difficult to separate from gas mixtures like natural gas. Metal organic frameworks have been widely studied for gas separation with high porosity and wide range of possible structures. In this study, selective binding of dinitrogen to the coordinatively unsaturated metal site in M-MOF-74 (M=Mg, V, Cr, Mn, Fe, Co, Ni, Cu) under external electric field is investigated with density functional theory. External electric field applied to the metal site enhance π*-backbonding between the transition metal and dinitrogen while weakening σ-bond between the metal and other small gas molecules. Amongst aforementioned 3d transition metals except Vanadium, Co-MOF-74 and Fe-MOF-74 show the highest dinitrogen binding energy, twice higher than that of methane and carbon dioxide. We suggest these two frameworks for dinitrogen selective separation process such as N_2/CH_4, N_2/CO_2 by applying external electric field.