ADSORPTION ON ZEOLITES

THE JOURNAL OF PHYSICAL CHEMISTRY C

IF= 4.520

Combined Experimental and Theoretical Investigations of Heterogeneous Dual Cation Sites in Cu,M-FER Zeolites

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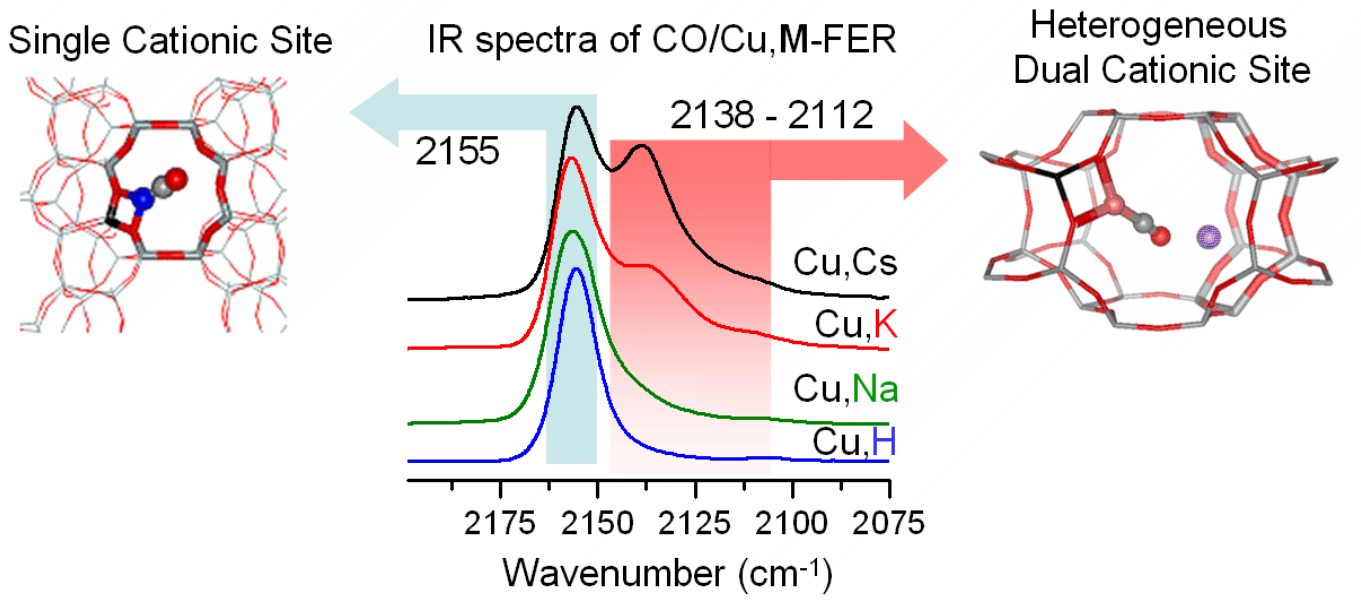
J. Phys. Chem. C, 2011, 115 (27), pp 13 312-13 321



Abstract: IR spectra of carbonyl species are usually understood within a concept of CO adsorption on a single cation site (SCS). However, when the concentration of extra-framework metal cations in microporous materials increases, the CO molecule may interact with two cations in the same time. Recently, bridged M^+···CO···M^+ complexes were found and described at atomic scale level in alkali metal exchanged FER and MFI zeolites. This finding prompted the question of whether similar complexes would also occur in zeolites with other cations and whether they can be behind some peculiar features of some IR spectra or peculiar adsorption behavior. The concept of dual cation sites is extended for the situation where CO is strongly bound on the Cu^+ cation and it also interacts with the extra-framework alkal-metal cation. The existence and properties of the CO adsorption complexes on such *heterogeneous* dual cation sites are discussed for Cu,M-FER zeolites (M = H, Na, K, Cs) having various compositions. Based on a good agreement between theoretical (perdiodic density functional theory) and experimental (IR, microcalorimetry, TPD) results the interpretation of some IR features is offered.