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BOOK OF ABSTRACTS

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Mobilities of heavier alkali cations (Me = K, Rb, Cs) as the key for high CO_2 reactivities in FAU type zeolites

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Interplay of an available space for reaction center and mobility of alkali cations leads to crucial role of cell parameters for accurate calculation of activation barrier of CO_2 hydration in optimized MeX zeolite cells (Me = K, Rb, Cs) after Me cation exchange. While the CO_2 hydration is modeled in the MeX forms (Me = K, Rb, or Cs) with a fixed volume of NaX one, barrierless reaction is predicted for Me = Rb or Cs that is not confirmed by experimental data. If cell parameters are optimized with VASP according to the new Me cations after Na/Me exchange, Me = Rb or Cs, small activation energy is obtained in agreement with room temperature conditions of the CO_2 hydration. Earlier [1], heats of CO_2 hydration in optimized MeY zeolite cells showed thermodynamic allowance of hydration for K and Cs (small positive heats for K or small negative heats for Cs compared to high positive heats for Li and Na) in agreement with IR data [2]. All the data for MeX and MeY zeolites are discussed together regarding 3- or 2-cation reaction centers in MeX and 3- or 4-cation sites with obtained hydrocarbonate in MeY, Me = K, Cs.

[1] A.V. Larin, Microporous Mesoporous Mater. 228 (2016) 182-195 [2] G.D. Pirngruber, P. Raybaud, et al., Phys. Chem. Chem. Phys., 2010, 12, 13534