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Francesca Bleken, Stian Svelle, Karl Petter Lillerud, Unni Olsbye, Bjørnar Arstad, and Ole Swang*: Thermochemistry of Organic Reactions in Microporous Oxides by Atomistic Simulations: Benchmarking against Periodic B3LYP

Page 7391. The calculations were carried out using CASTEP as implemented in the Materials Studio 4.4 package. Meanwhile, an error in the implementation of the B3LYP functional in CASTEP present in MS4.4 has been identified, and in Materials Studio 5.5 (MS5.5), the error has been corrected. A repetition of the single point calculations in CASTEP/B3LYP was thus in order. The CASTEP results for both MS4.4 and MS 5.5 are shown in Table 1, and they show that both adsorption energies

TABLE 1: Adsorption (ΔE_{ads}) and Activation ($\Delta E^{\ddagger}$) Energies (kJ/mol) for the Single Point CASTEP/B3LYP Performed with MS4.4 and MS5.5

	version of material studio		
	MS4.4	MS 5.5	Δ
ΔE_{ads} SSZ−OH	−98	−79	19
ΔE_{ads} SAPO−OH	−81	−59	22
ΔE_{ads} SSZ-Cl	−25	−12	13
ΔE_{ads} SAPO-Cl	−15	−6	9
$\Delta E^{\ddagger}$ SSZ−OH	156	169	−13
$\Delta E^{\ddagger}$ SAPO−OH	162	171	−9
$\Delta E^{\ddagger}$ SSZ-Cl	107	137	−30
$\Delta E^{\ddagger}$ SAPO-Cl	118	148	−30

and activation energies changed. However, our qualitative conclusions are not affected by the new results: A stronger sorption of methanol compared to methyl chloride is predicted in both structures, and a lower activation barrier for methyl chloride than for methanol. Also, both sorbates interact more strongly with SSZ-13 than with SAPO-34, in line with the latter having weaker acid sites. Differences in activation barriers between the two materials are not very pronounced, in line with the results obtained with MS4.4.

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