

Modeling Ammonia and Water co-Adsorption in Cu^I-SSZ-13 Zeolite Using DFT Calculations

Hugo Petitjean¹, Céline Chizallet² and Dorothée Berthomieu^{1}*

¹Institut Charles Gerhardt Montpellier, UMR 5253 CNRS-ENSCM-UM, Montpellier, France

²IFP Energies Nouvelles, Rond-point de l'échangeur de Solaize, BP3, 69360 Solaize, France

Table S1. Cu^I in exchange positions I, IV and IV' in SSZ-13: B3LYP relative energies of with respect to the most stable structure **A** (in kJ.mol⁻¹)

Structure label	Cu ^I position	Relative energy /kJ.mol ⁻¹
A	I	0
B	IV	43
C	IV'	54

Table S2. Cu^I in exchange positions I, IV and IV' in SSZ-13: B3LYP geometry parameters calculated for **A**, **B** and **C** (Figure 1). Bond distances are in Å.

	Site I	Site IV	Site IV'
Bonds	A	B	C
Si-O ₁	1.623	1.626	1.626
Si-O ₂	1.606	1.614	1.619
Si-O ₃	1.618	1.624	1.615
Si-O ₄	1.646	1.625	1.622
Cu-O ₁		2.046	
Cu-O ₂		2.332	2.122
Cu-O ₃		2.236	2.065
Cu-O ₄	2.003		
Cu-O ₄	2.090		
Cu-O ₄	2.189		
Cu...Al	3.053	2.847	2.764
Al-O ₁	1.715	1.693	1.702
Al-O ₂	1.687	1.805	1.756
Al-O ₃	1.720	1.713	1.771
Al-O ₄	1.798	1.722	1.702

Table S3. Adsorption structures of 2 NH₃ in Cu^I-SSZ-13 unit cell: B3LYP and B3LYP-D* relative energies (kJ/mol) and geometry parameters (Å) for the optimized structures of (NH₃)₂Cu^I-SSZ-13 **X**, **Y** and **Z** (Figure 2).

	X	X B3LYP- D*	Y	Z
Si-O ₁	1.628	1.609	1.621	1.621
Si-O ₂	1.616	1.629	1.621	1.621
Si-O ₃	1.614	1.620	1.619	1.619
Si-O ₄	1.622	1.618	1.624	1.624
Cu-O ₁			2.730	
Cu-O ₂			3.332	2.554
Cu-O ₃			3.258	3.286
Cu-O ₄	4.487			
Cu-O ₄	5.099			
Cu-O ₄	3.701	3.462		
Cu-N	1.939	1.948	1.946	1.953
Cu-N	1.940	1.948	1.950	1.954
Cu...Al	4.348	4.283	3.819	3.278
Al-O ₁	1.739	1.737	1.738	1.738
Al-O ₂	1.719	1.718	1.724	1.724
Al-O ₃	1.737	1.727	1.729	1.729
Al-O ₄	1.726	1.736	1.718	1.718
Relative energies (kJ.mol ⁻¹)	0		19	34

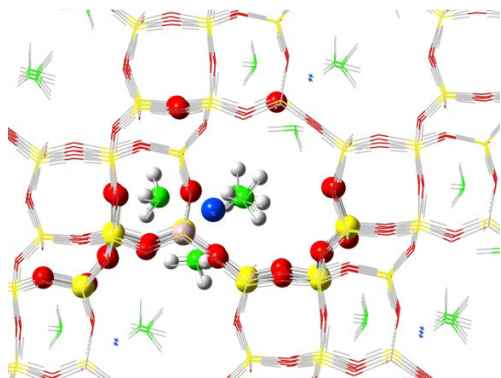
Table S4. Adsorption of H₂O or NH₃ on Cu^I-SSZ-13: B3LYP-D* cumulated adsorption energies (in kJ/mol) and coordination number CN (defined as the number of heavy atoms within 2.3 Å of Cu²⁴). (n,m) are labels for the configurations with n water molecules and m ammonia molecules (0≤n≤4 and 0≤m≤4).

(n, m)	H ₂ O number/CN	Cumulated H ₂ O adsorption energy (kJ/mol)	(n, m)	NH ₃ number/CN	Cumulated NH ₃ adsorption energy (kJ/mol)
(0,0)	0/3	0	(0,0)	0/3	0
(1,0)	1/2	-87	(0,1)	1/2	-111
(2,0)	2/2	-168	(0,2)	2/2	-265
(3,0)	3/3	-172	(0,3)	3/3	-308
(4,0)	4/4	-223	(0,4)	4/4	-336

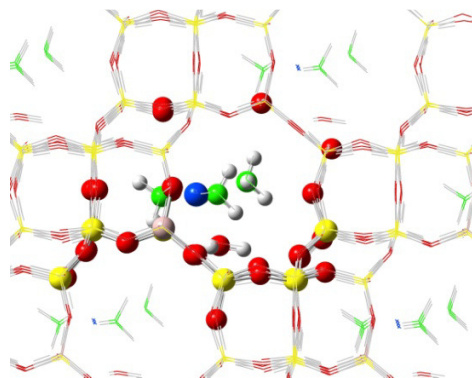
Table S5. Adsorption and co-adsorption of H₂O and NH₃ on Cu^I-SSZ-13: B3LYP-D* geometry parameters calculated for the 14 most stable structures with (n, m) configurations (n water molecules, m ammonia molecules with (0≤n≤4 and 0≤m≤4)). Cu^I is located in the channel of the 8MR in each (n,m) configuration.

(n,m) configurations	Ligand number/CN	Cu-L Bond lengths (Å)	Cu...Al Distance (Å)
(0,4)	4/4	2.153 2.200 2.254 2.149	4.806
(1,3)	4/3	2.210 2.028 2.004 3.050 (Cu-O)	4.748
(2,2)	4/2	1.960 1.963 2.515 (Cu-O) 3.746 (Cu-O)	3.908
(3,1)	4/2	1.950 1.935(Cu-O) 2.504(Cu-O) 3.512 (Cu-O)	3.845
(4,0)	4/4	2.073 2.055 2.331 2.274	4.958
(0,3)	3/3	2.001 2.017 2.256	4.503
(1,2)	3/2	1.966 1.968 2.401(Cu-O)	4.805
(2,1)	3/2	1.970 1.989 (Cu-O) 2.405 (Cu-O)	4.492
(3,0)	3/3	1.986 (Cu-O) 2.036 (Cu-O) 2.263 (Cu-O)	3.382
(0,2)	2/2	1.948 1.947	4.283

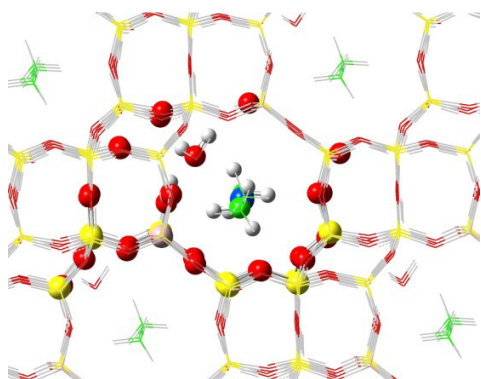
(1,1)	2/2	1.947	
		1.921 (Cu-O)	4.146
(2,0)	2/2	1.925 (Cu-O)	
		1.926 (Cu-O)	4.344
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(0,1)	1/1	1.980	3.400
(1,0)	1/1	1.914	4.275
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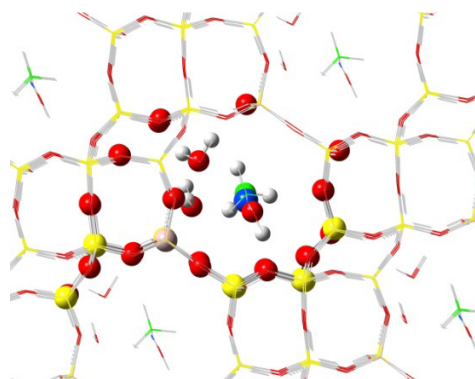
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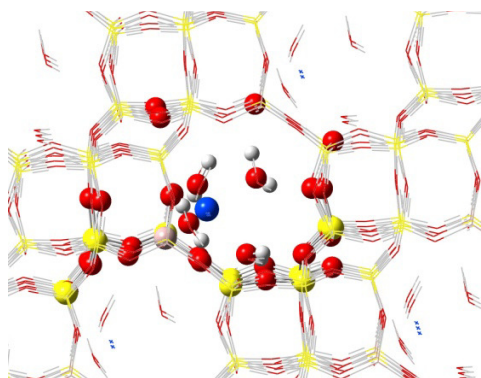
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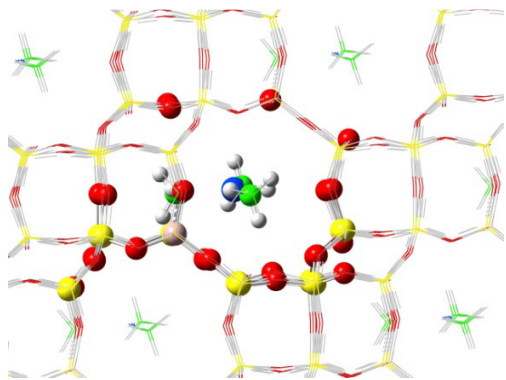
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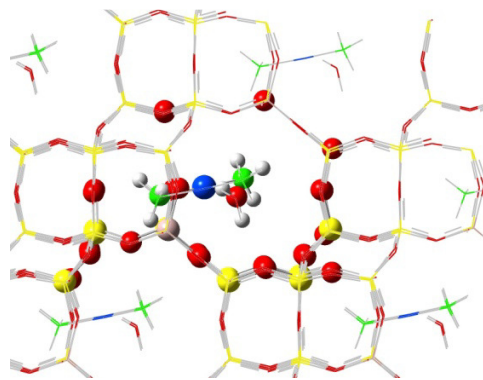
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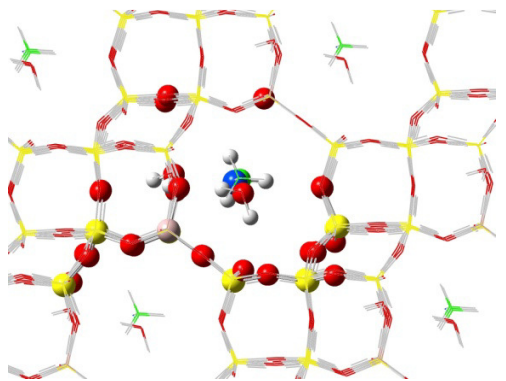
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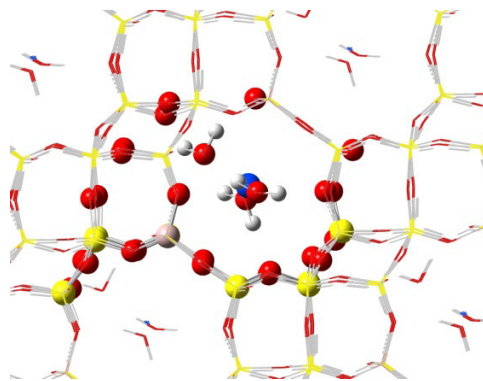
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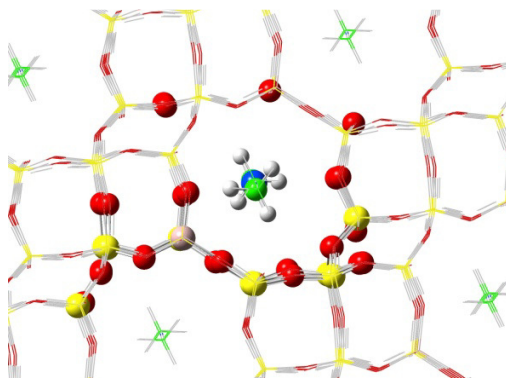
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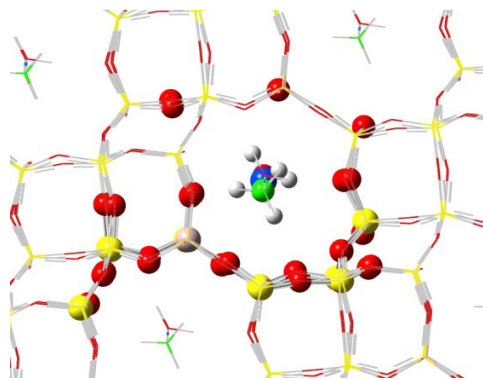
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(3,0)



(0,2)



(1,1)

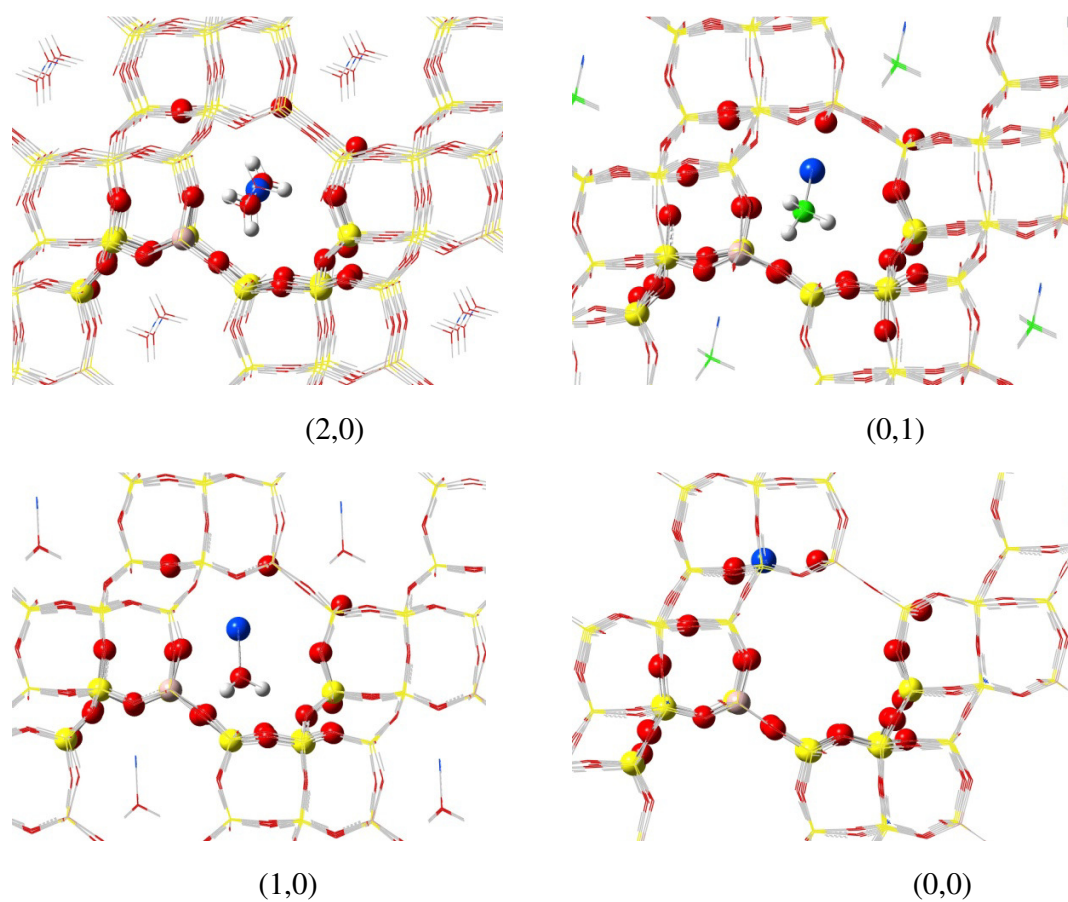


Figure S1. Adsorption and co-adsorption of H₂O and NH₃ on Cu^I-SSZ-13: views of the optimized geometries for the adsorption of n H₂O and m NH₃ on Cu^I-SSZ-13 (labeled as (n, m) with $0 \leq n \leq 4$ and $0 \leq m \leq 4$). Red balls are O, yellow balls are Si, rose ball is Al, blue ball is copper, white balls are H and green balls are N.