Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information 1

Relative stability of SCM-14 germanosilicate with different distribution of germanium ions in absence and presence of structure-directing agents

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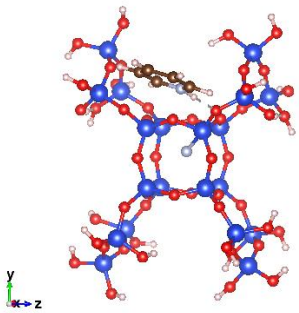

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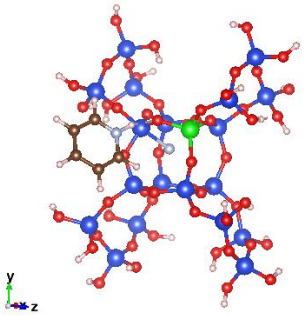

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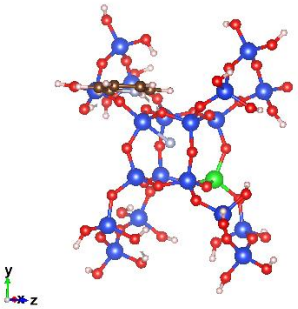

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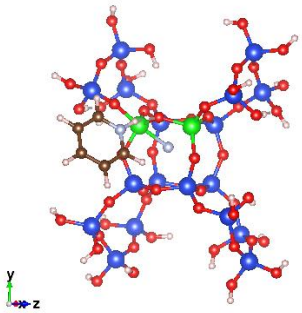

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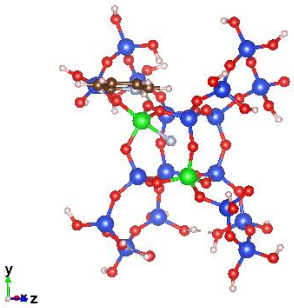

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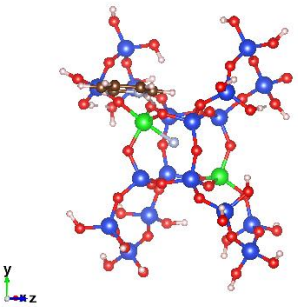

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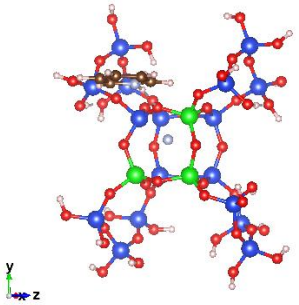

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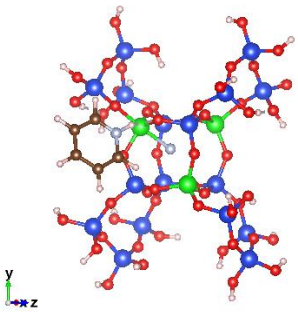

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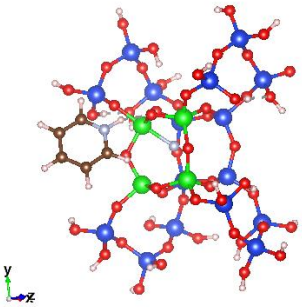

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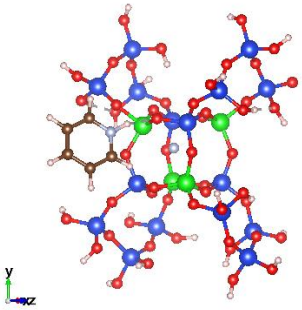

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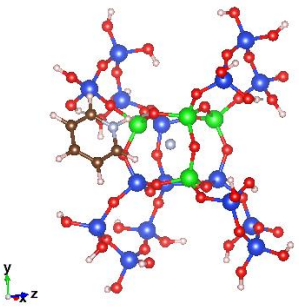

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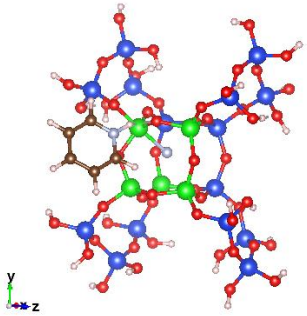

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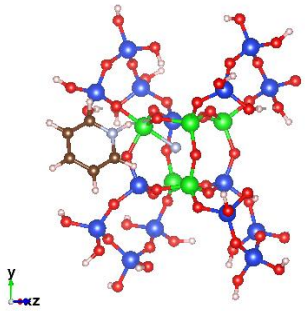

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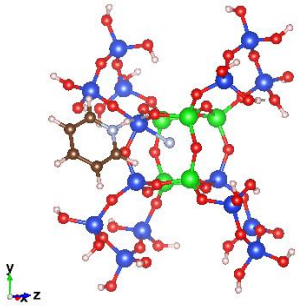

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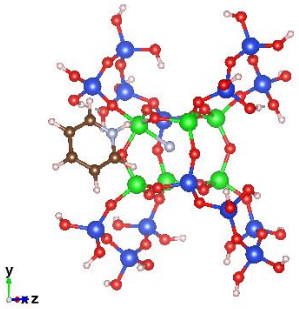

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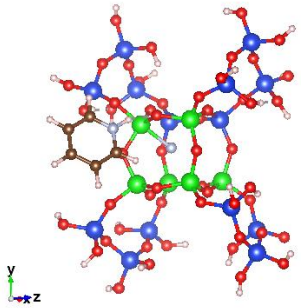

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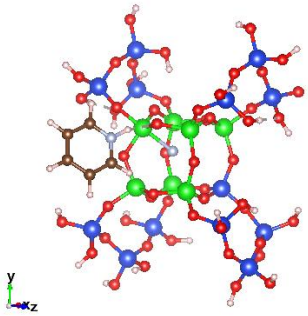

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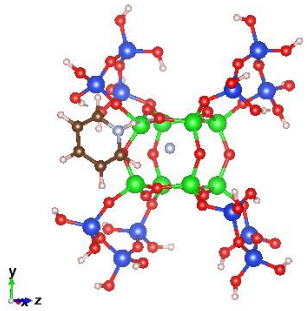


D4R(8Ge)

Figure S1. Structures used for simulation of ^{19}F NMR chemical shifts of fluorine inside D4Rs with different germanium content and distribution: Ge in green, F in white. Figures are generated with VESTA, ver. 3.4.3.

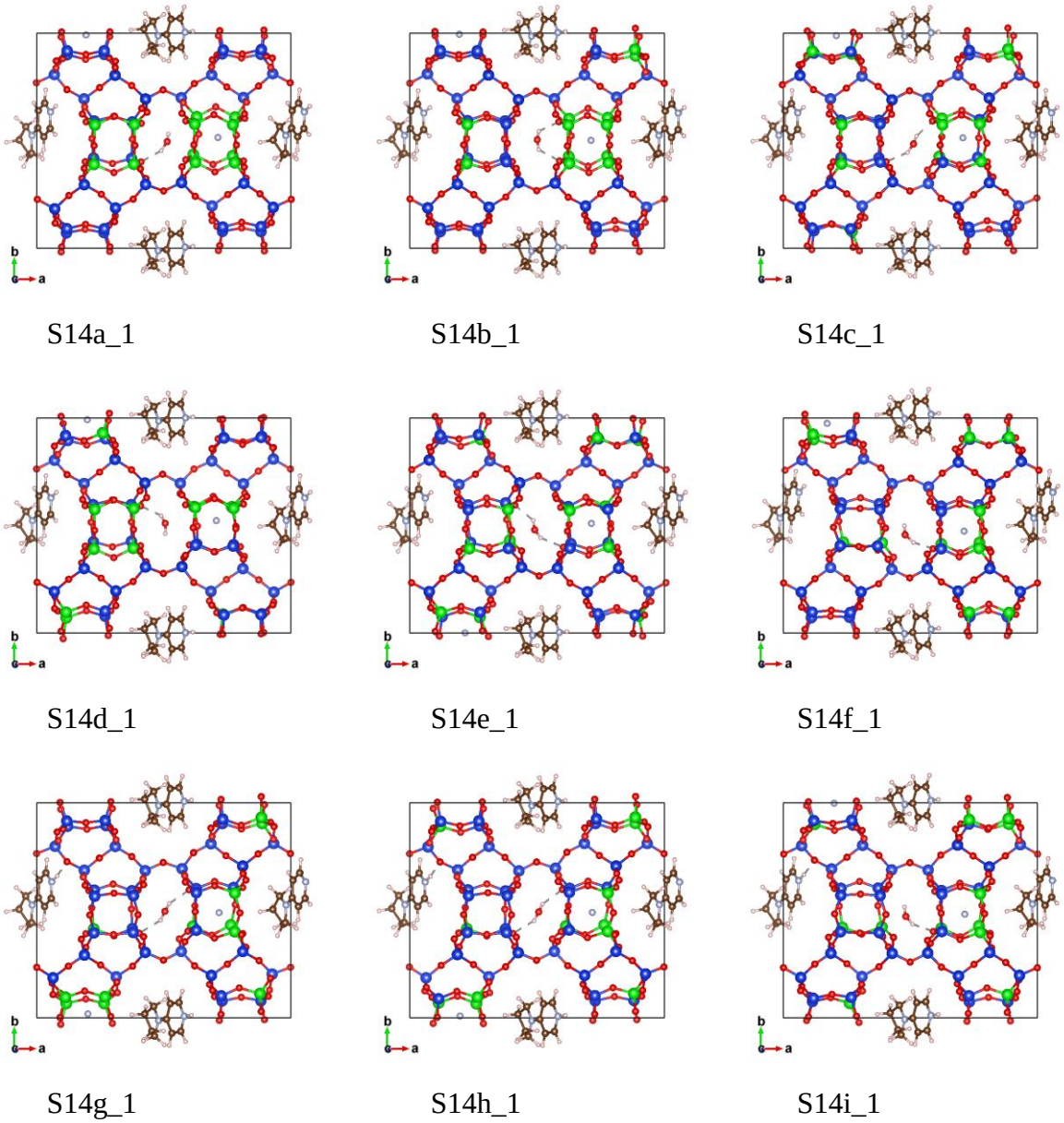
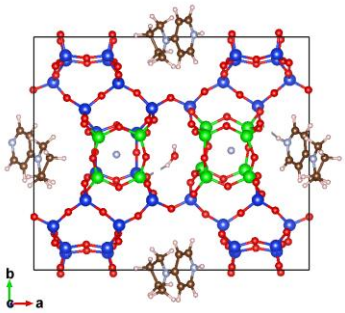
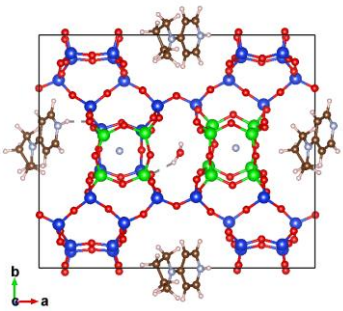


Figure S2. Optimized structures of the models containing SDA – series 1 (notation of the structure is shown below each figure). Color coding: Si-blue, O-red, Ge-green, C-brown, N-light grey, H-pink, F-light blue.



S14a_2



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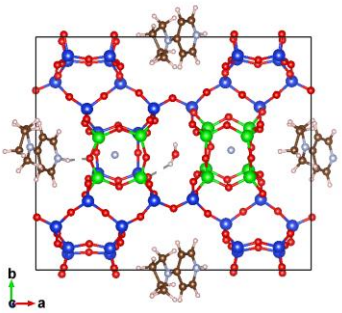

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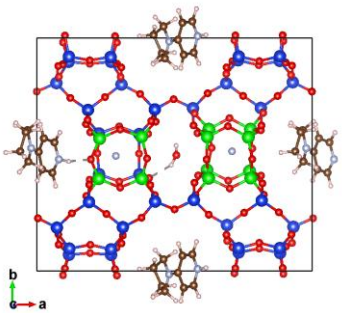

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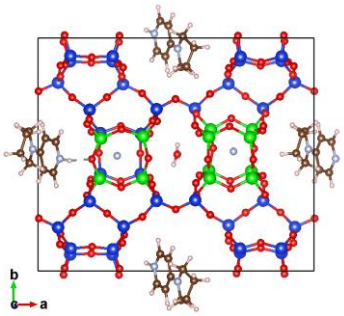

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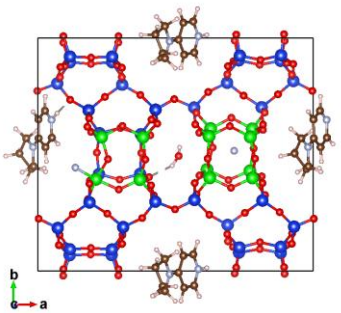

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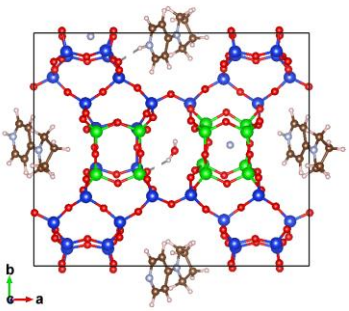

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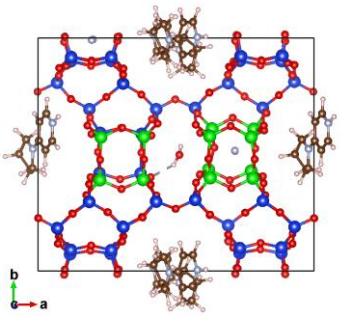

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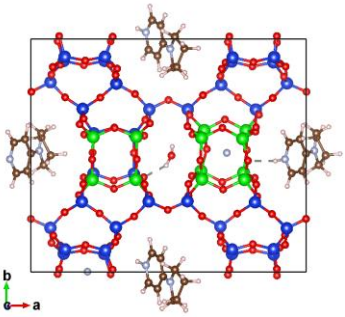

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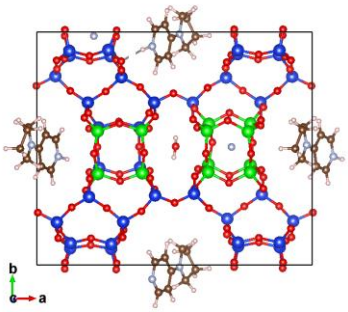

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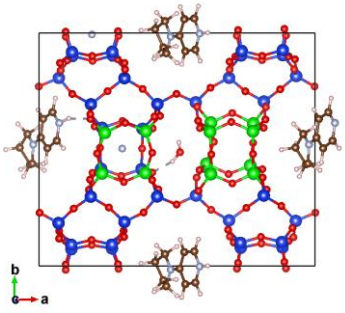

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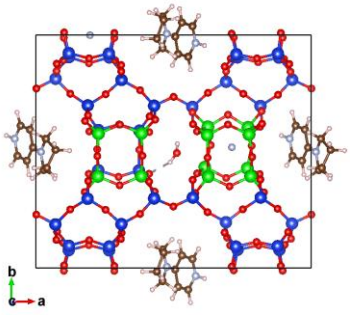

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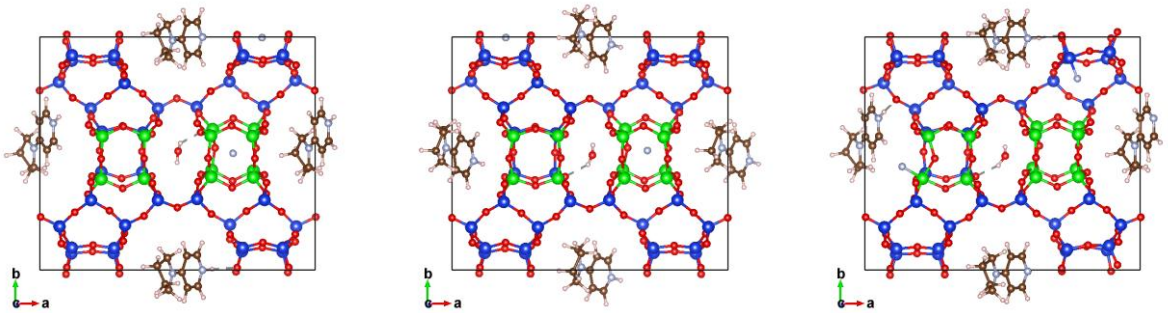
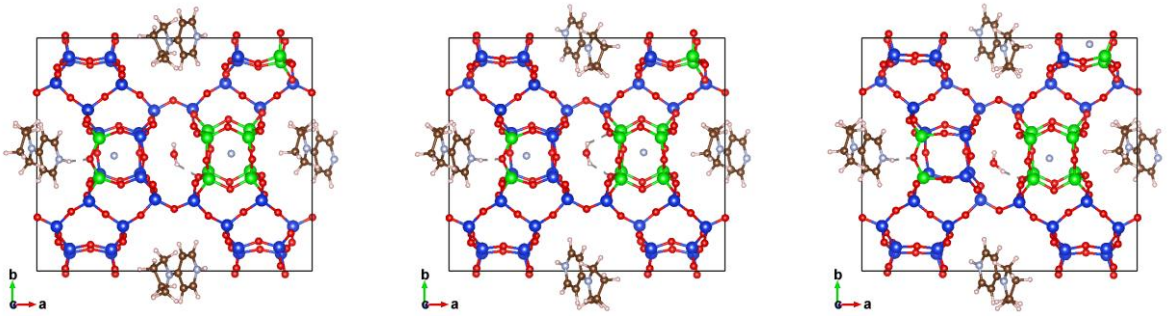
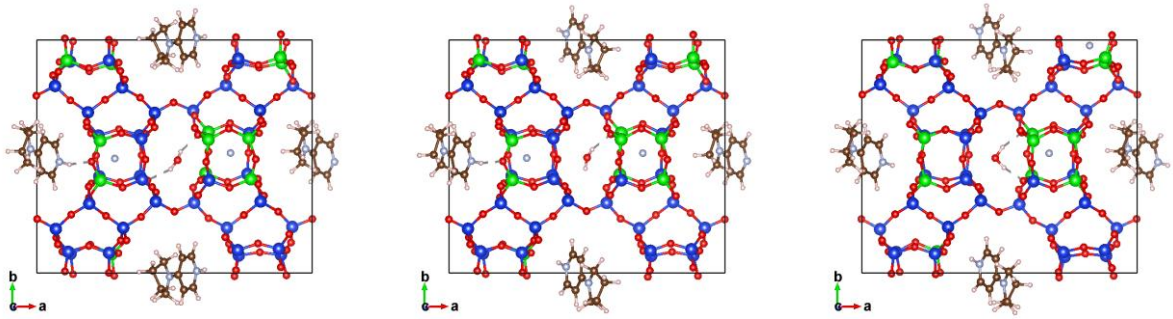


S14a_14 S14a_15 S14a_16

Figure S3. Optimized structures of the models containing SDA – series 2 (notation of the structure is shown below each figure). Color coding: Si-blue, O-red, Ge-green, C-brown, N-light grey, H-pink, F-light blue. Note that model S14a_1 is the same as in series 1.



S14b_4 S14b_6 S14b_17



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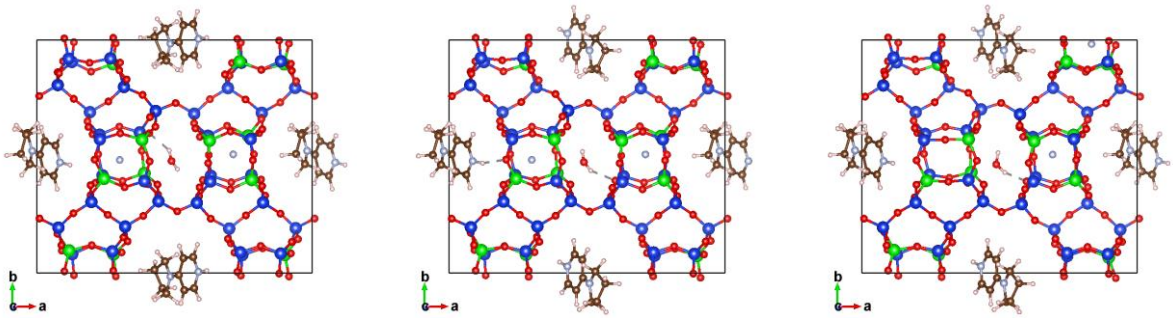
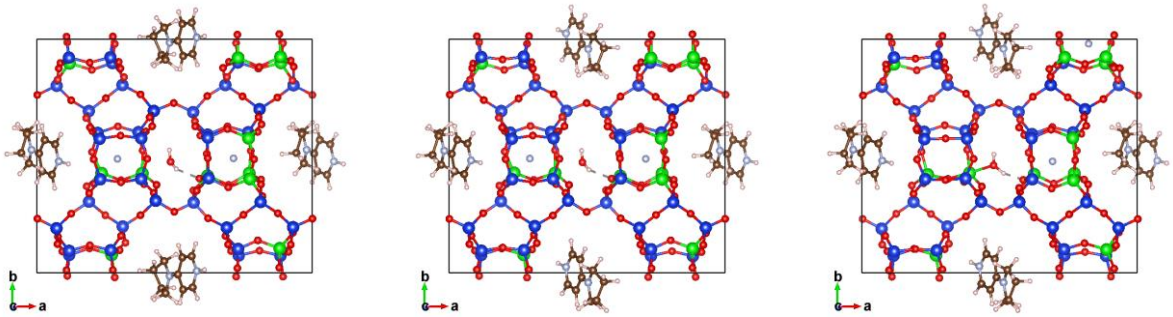
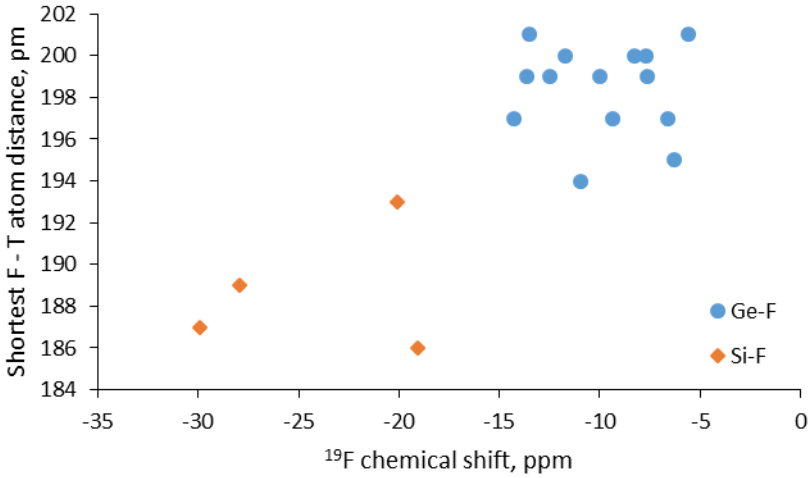


S14e_4 S14e_6 S14e_17



S14i_4 S14i_6 S14i_17

Figure S4. Optimized structures of the SCM-14 models containing SDA – series 2 (notation of the structure is shown below each figure). Color coding: Si-blue, O-red, Ge-green, C-brown, N-light grey, H-pink, F-light blue. Note that model s142j_2h_22d is the same as the model s142j_2d of series 1.



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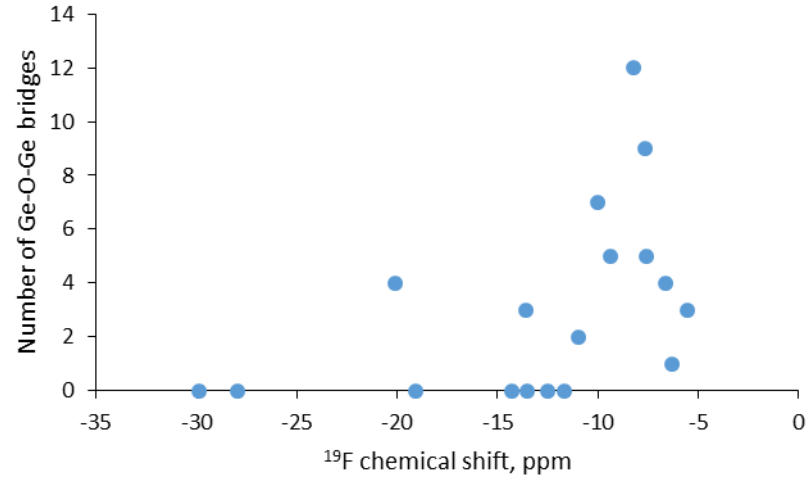

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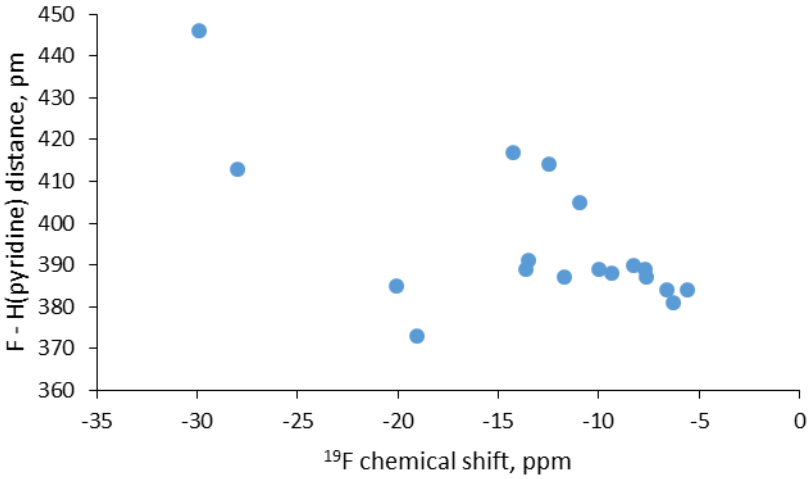
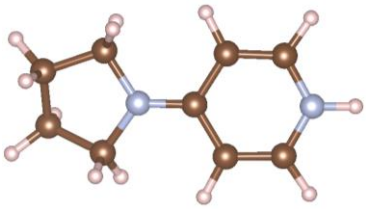
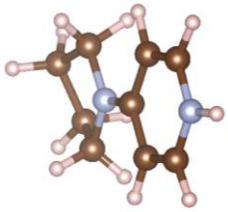


C

Figure S5. Plots of the calculated values for ^{19}F NMR chemical shift for fluoride anion in D4Rs with different content and distribution of Ge: A: shortest T atom – F distance (in pm), B: number of Ge-O-Ge bridges in the D4R model, C: distance between fluorine and the proton from the protonated pyridine (in pm).





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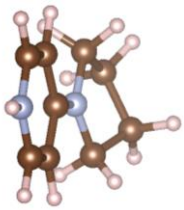

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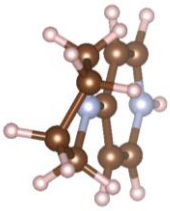

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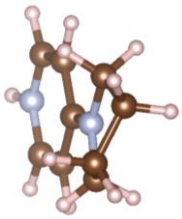

bl

Figure S6. Structure of protonated 4-pyrrolidinopyridine and notation of its orientation inside the channels of SCM-14 zeolite.