Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information:

Hydroxylation of silica nanoclusters $(SiO_2)_M(H_2O)_N$ M=4, 8, 16, 24: stability and structural trends

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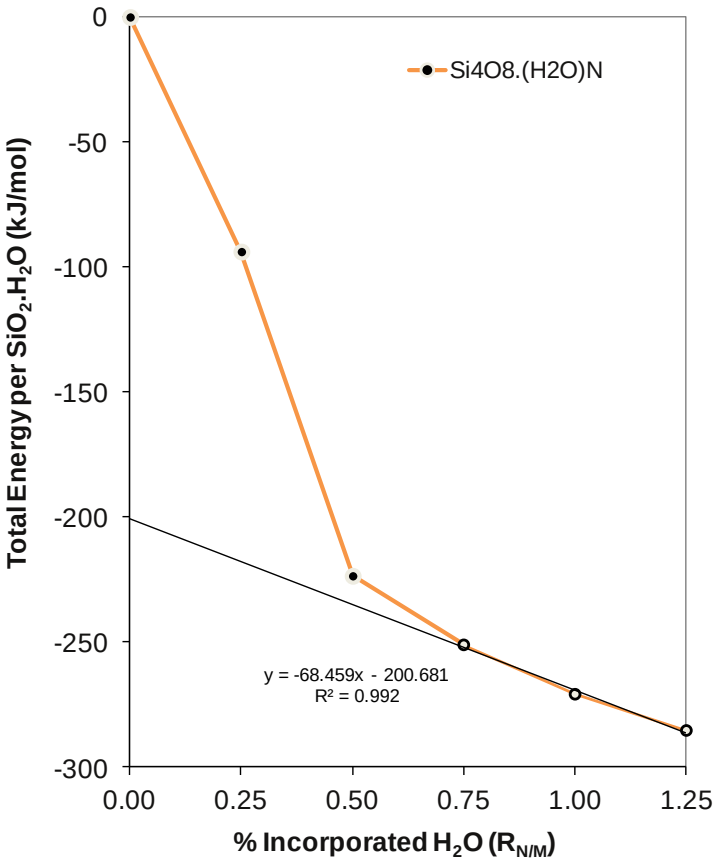
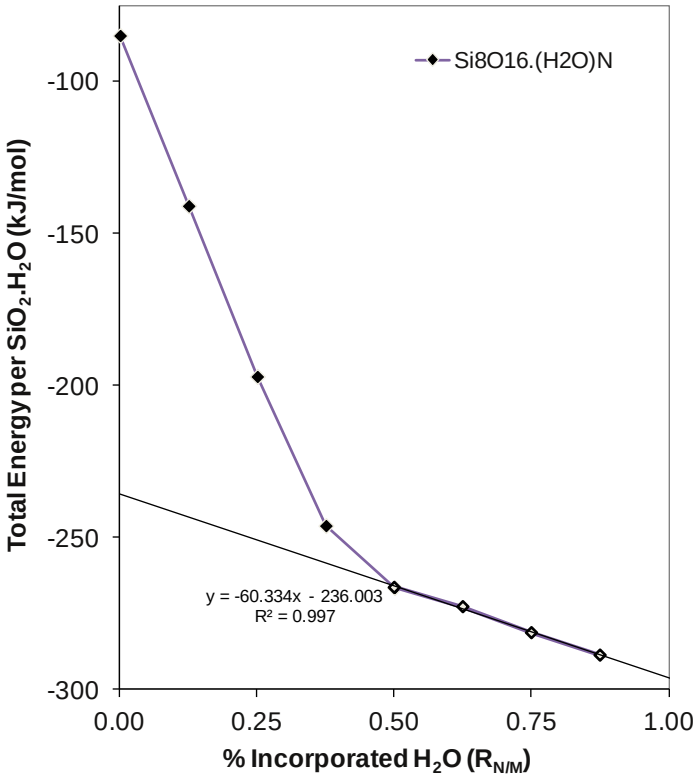
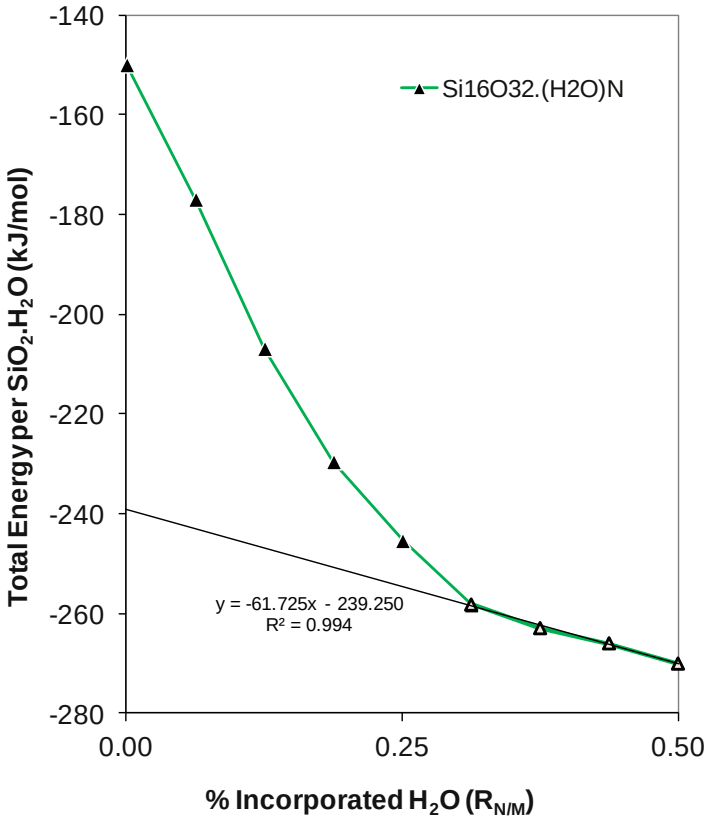
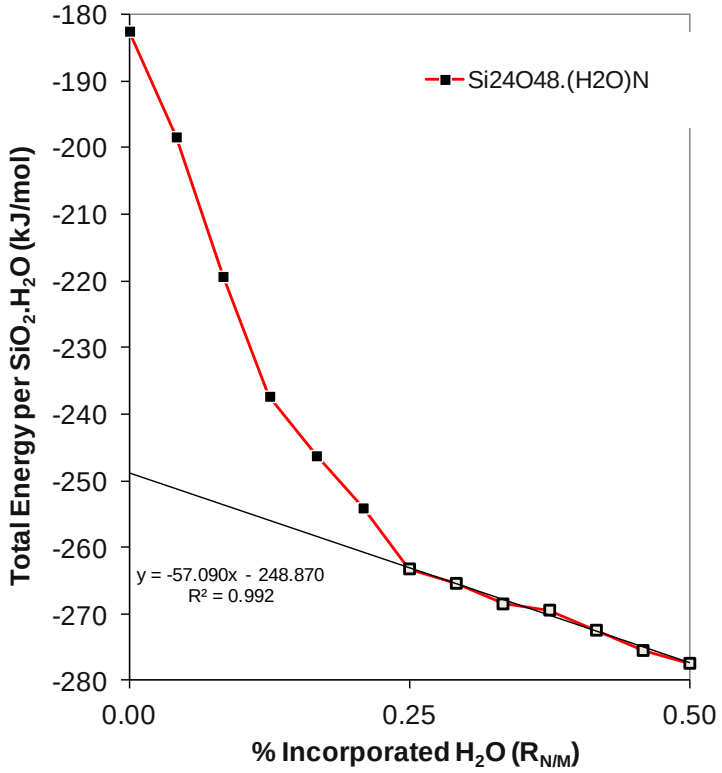
1. Linear fits to the open data points in Figure 3.

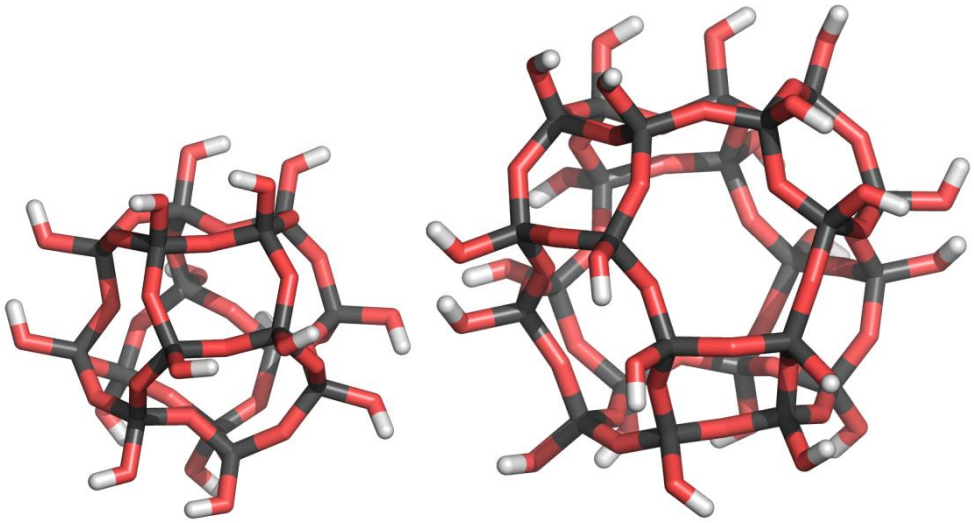






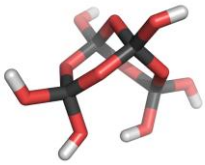


2. Structures of the lowest energy $R_{N/M}$=0.5 cage-like clusters found for M=16 (left) and 24 (right).

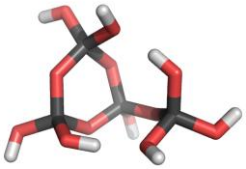


3. Structures of the lowest energy $(SiO_2)_4(H_2O)_N$ and $(SiO_2)_8(H_2O)_N$ clusters found for $R_{N/M} \geq 0.5$.

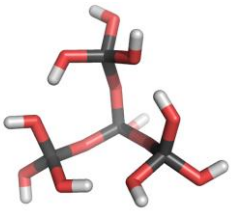
$(SiO_2)_4(H_2O)_2$
$R_{N/M}=0.5$



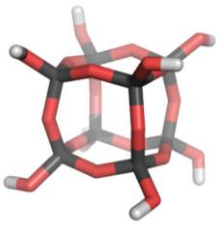
$(SiO_2)_4(H_2O)_3$
$R_{N/M}=0.75$



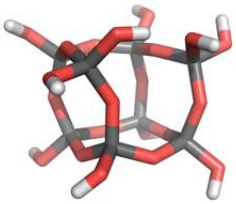
$(SiO_2)_4(H_2O)_4$
$R_{N/M}=1.0$



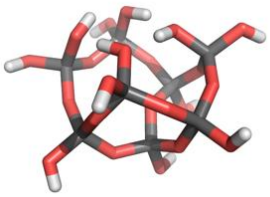
$(SiO_2)_4(H_2O)_5$
$R_{N/M}=1.25$



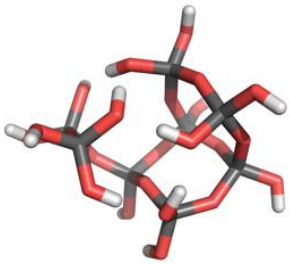
$(SiO_2)_8(H_2O)_4$
$R_{N/M}=0.5$



$(SiO_2)_8(H_2O)_5$
$R_{N/M}=0.625$



$(SiO_2)_8(H_2O)_6$
$R_{N/M}=0.75$



$(SiO_2)_8(H_2O)_7$
$R_{N/M}=0.875$