

Supplementary Materials

On the Sorption Mode of U(IV) at Calcium Silicate Hydrate: A Comparison of Adsorption, Absorption in the Interlayer, and Incorporation by Means of Density Functional Calculations

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Figures showing all sorption complexes of U(IV) in CSH according to Table 1 of the main text. For the labeling of sites see section Sorption Sites of the main text.

Surface:

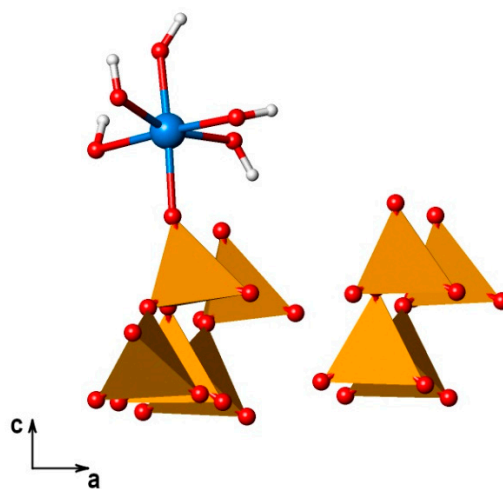


Figure S1. SiO.

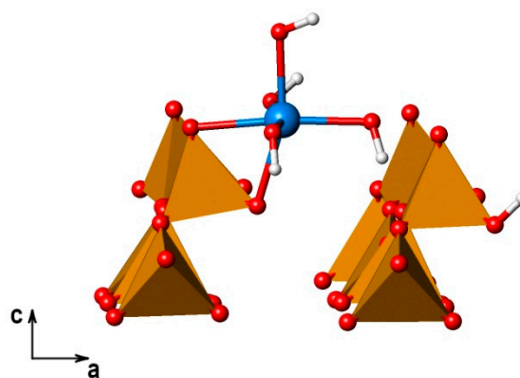


Figure S2. SiOO.

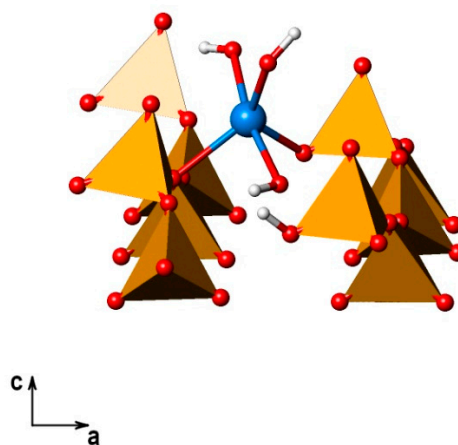


Figure S3. Chbr2.

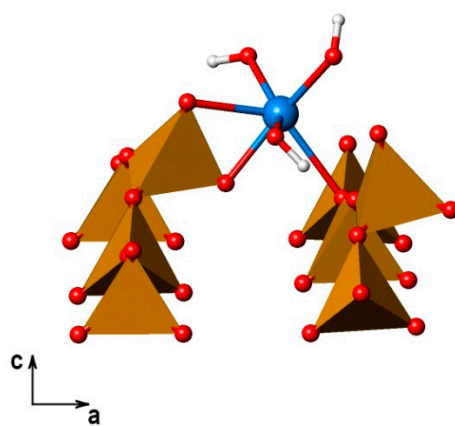


Figure S4. Chbr3.

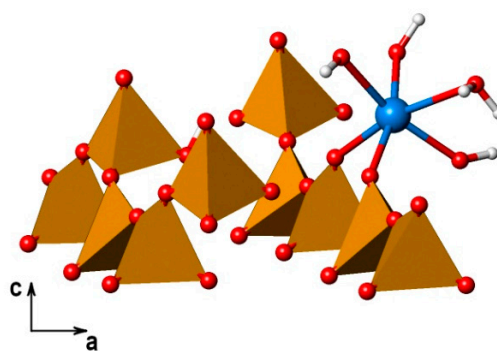


Figure S5. Def2.

Interlayer:

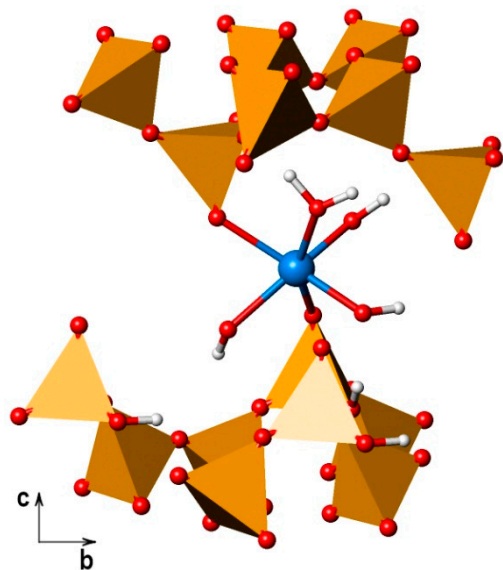


Figure S6. Lbr2.

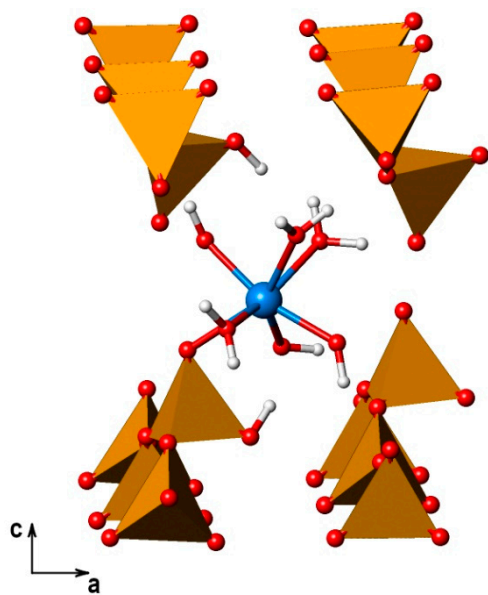


Figure S7. SiO.

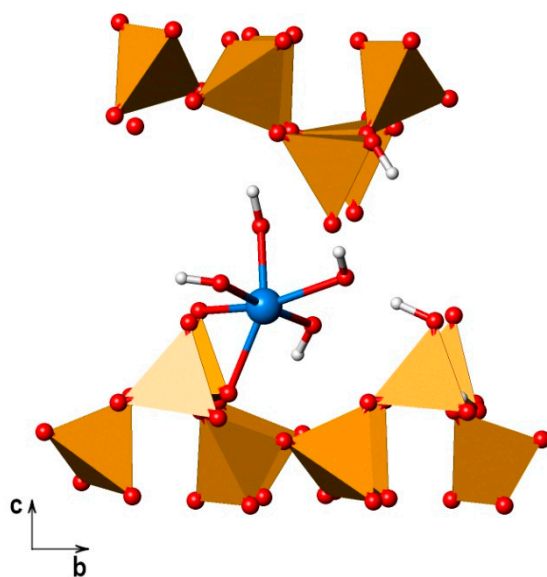


Figure S8. SiOO.

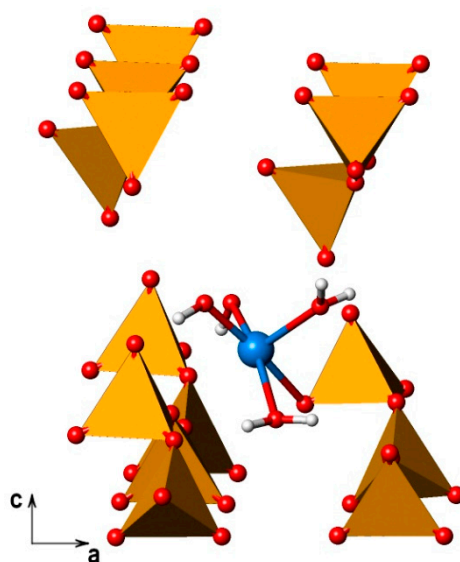


Figure S9. Chbr1.

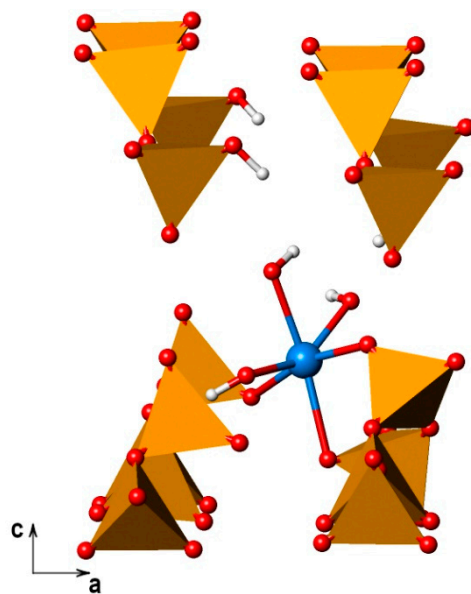


Figure S10. Chbr3.

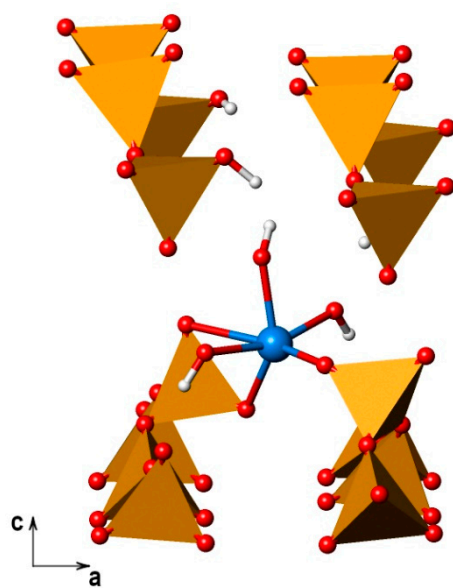


Figure S11. Chbr3'.

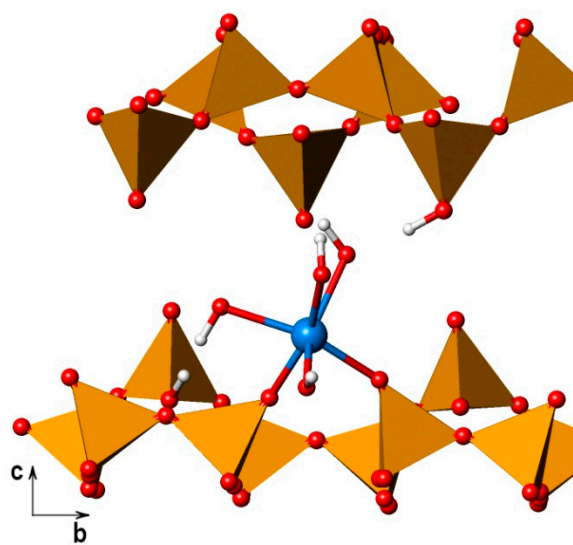


Figure S12. Def2.

CaO layer:

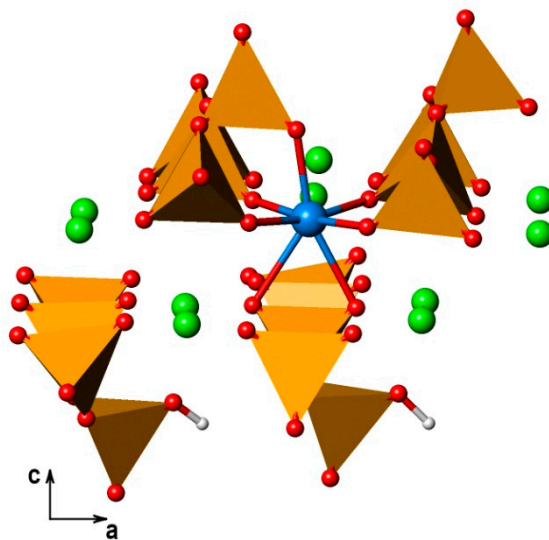


Figure S13. IncO7.

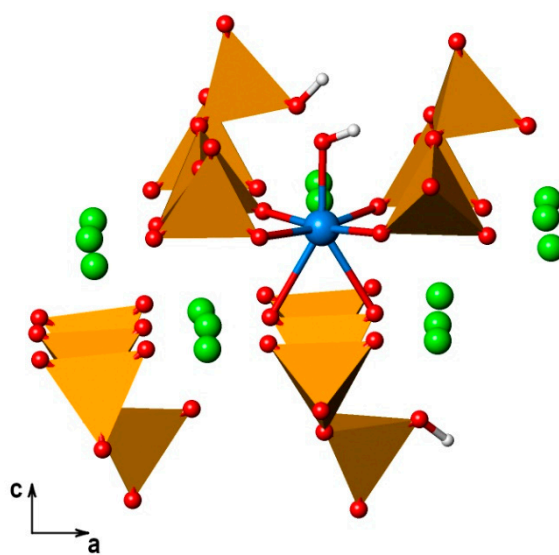


Figure S14. IncW7.