minerals

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Structure and Properties of Water in a New Model of the 10-Å Phase: Classical and Ab Initio Atomistic Computational Modeling

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Electronic Supplementary Material

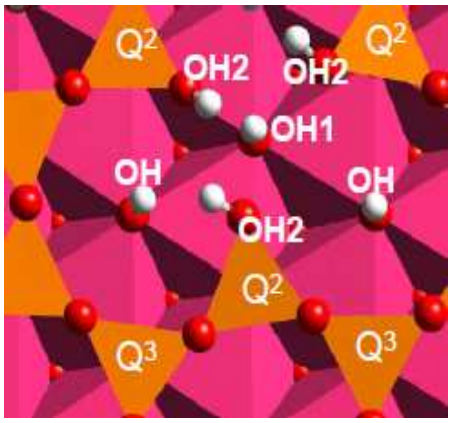
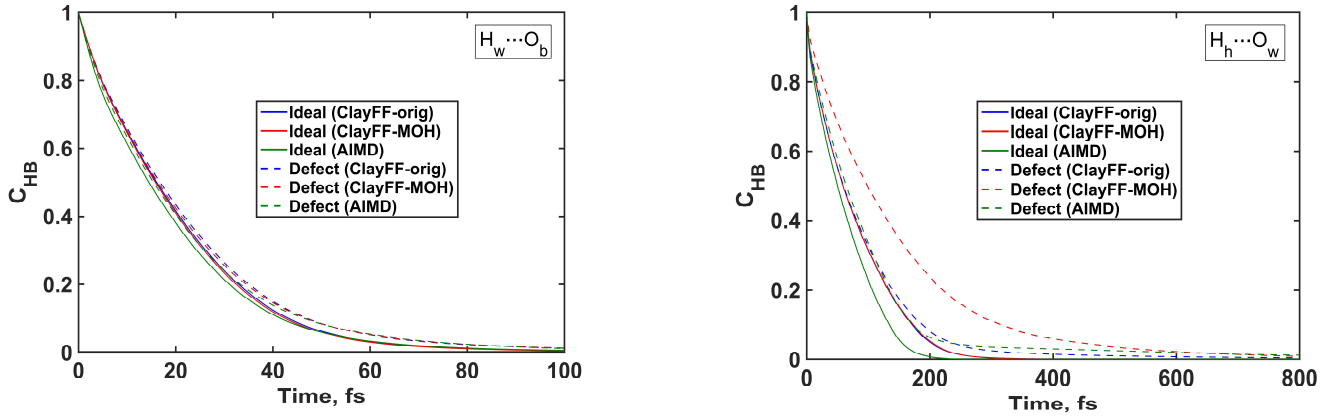


Figure S1. Q^3- and Q^2-type Si sites in the tetrahedral sheet of the TAP. (Here we are using the common notation for silicon-oxygen tetrahedra,Q^n where the superscript shows the number of other silicon-oxygen tetrahedra attached to the silicon tetrahedron under study [ref.S1,ref.S2]). OH—structural hydroxyls (Mg-O-H); OH1—hydroxyl inside in the defect (Mg-O-H); OH2—silanol groups (Si-O-H).

[ref.S1] Engelhardt, L. G.; Zeigan, D.; Jancke, H.; Wieker, W.; Hoebbel, D., ^{29}Si-NMR-Spektroskopie an Silicatlosungen. II. Zur Abhangigkeit der Struktur der Silicatanionen in wassrigen Natriumsilicatlosungen vom Na : Si-Verhaltnis. *Zeitschrift fur anorganische und allgemeine Chemie* **1975**, *418*, 17-28. https://doi.org/10.1002/zaac.19754180103

[ref.S2] Lippmaa, E.; Maegi, M.; Samoson, A.; Engelhardt, G.; Grimmer, A. R., Structural studies of silicates by solid-state high-resolution silicon-29 NMR. *J. Amer. Chem. Soc*. **1980**, *102*, 4889-4893. https://doi.org/10.1021/ja00535a008



(**a**) (**b**)

Figure S2. Continuous H-bonding time autocorrelation functions. **a** $H_w\cdots O_b$ pair; **b** $H_h\cdots O_w$ pair.

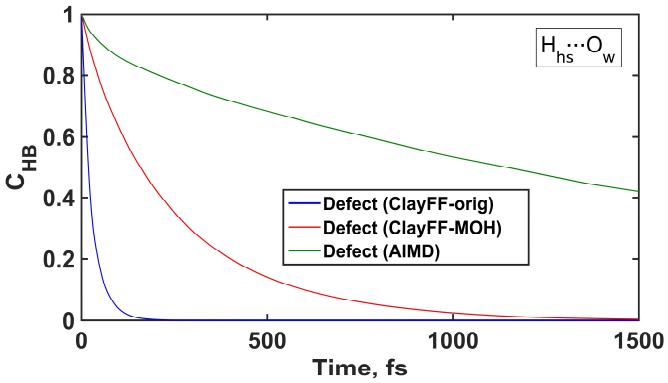


Figure S3. Continuous H-bonding time autocorrelation functions for the $H_{hs}\cdots O_w$ pairs.

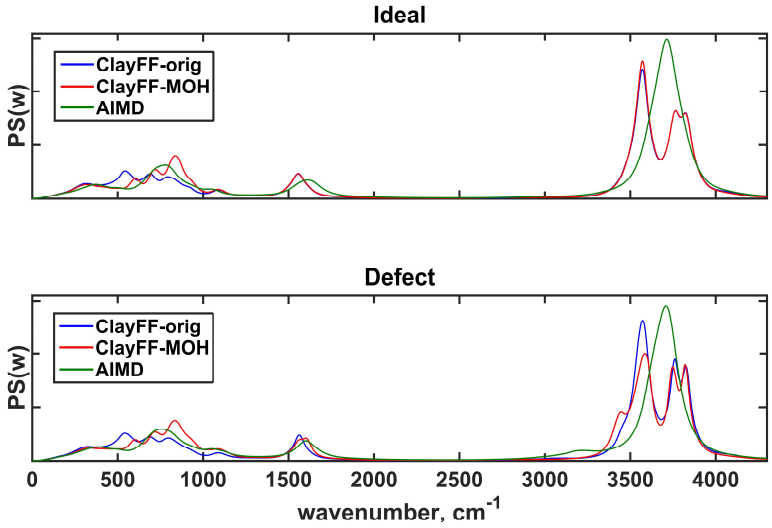


Figure S4. Total VDOS for the ideal and defect TAP models.

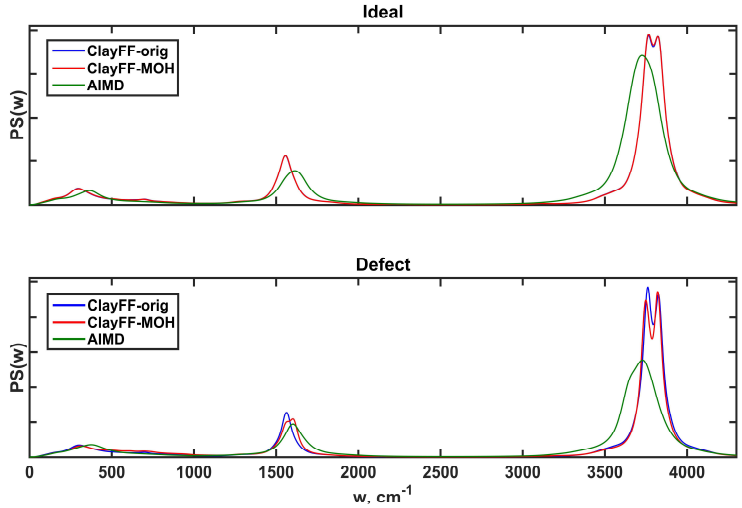


Figure S5. Partial VDOS of the interlayer H_2O molecules for the ideal and defect TAP models.

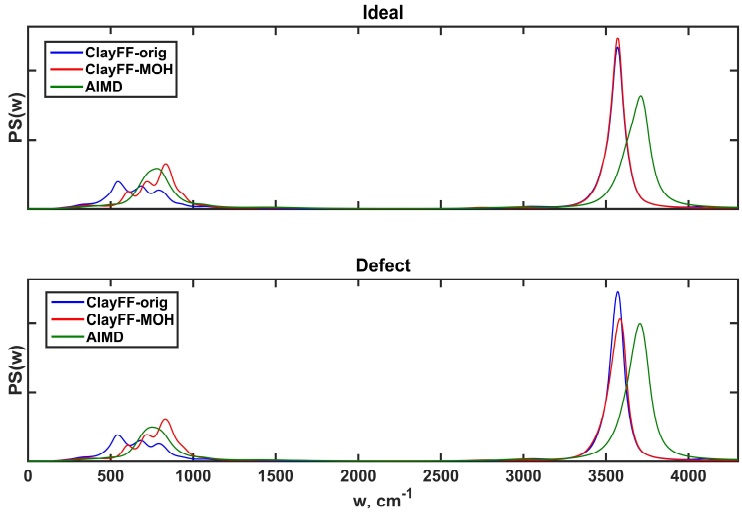


Figure S6. Partial VDOS of the H_h atoms for the ideal and defect TAP models.