

Supplementary materials

Water structure and dynamics in microporous mordenite

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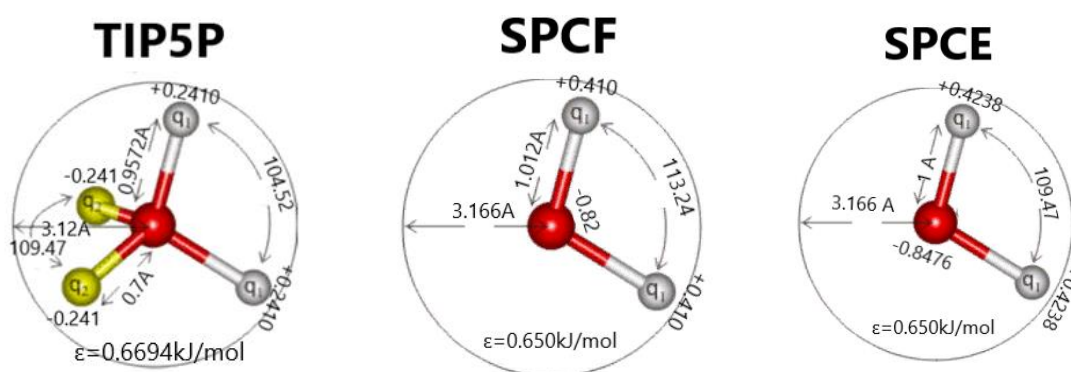
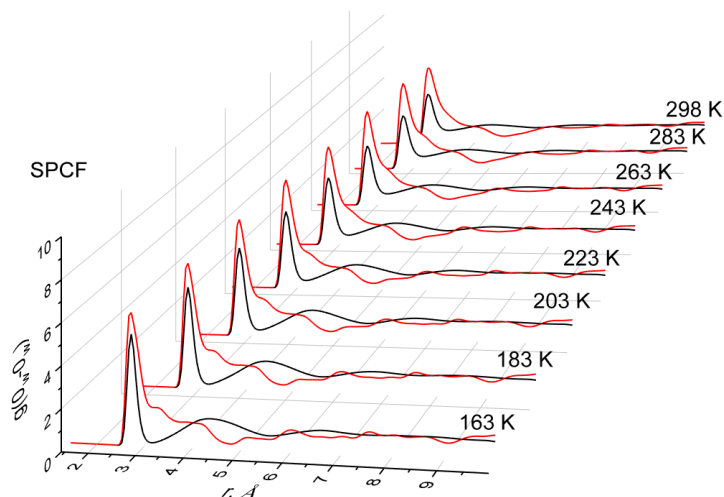


Fig. S1. Schematic representation of the water models used.



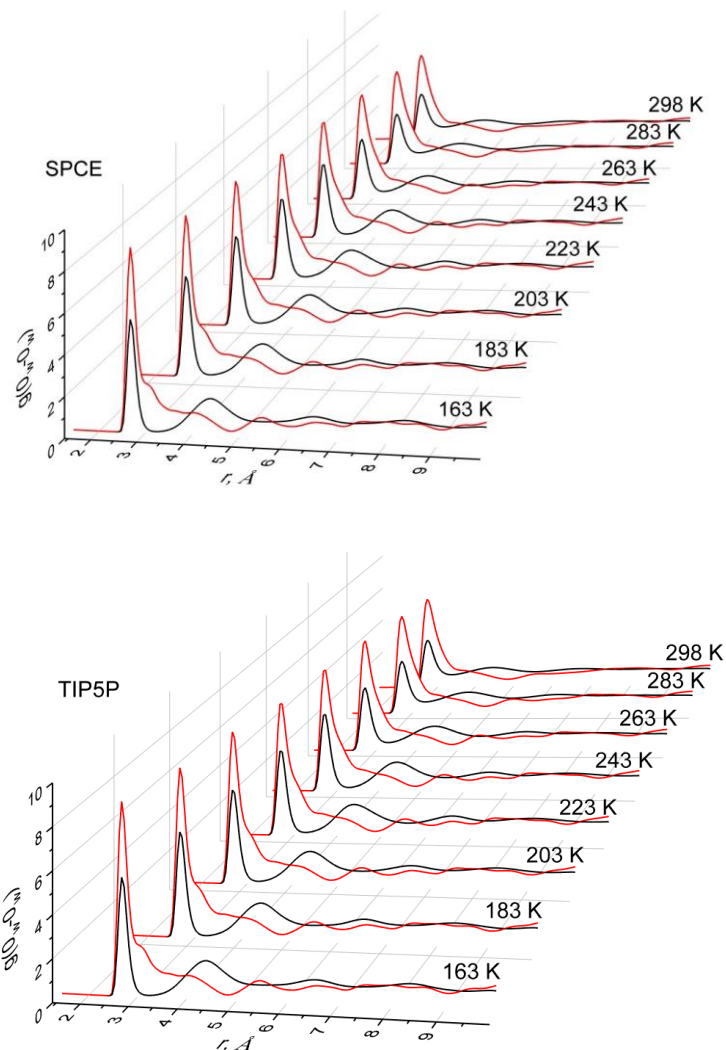


Fig. S2. Radial distribution functions between water oxygen atoms in bulk water (black line) and in mordenite pores (red) over a temperature range from 298 to 163 K

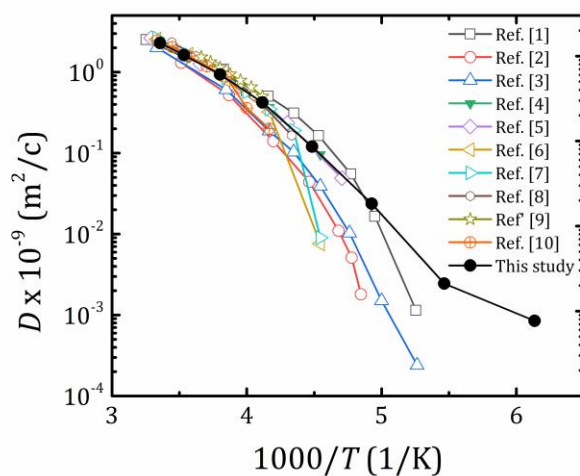


Fig. S3. Temperature dependence of self-diffusion coefficient for bulk SPCE water. Filled circles correspond to the present study, open symbols are data from Refs. [1–10].

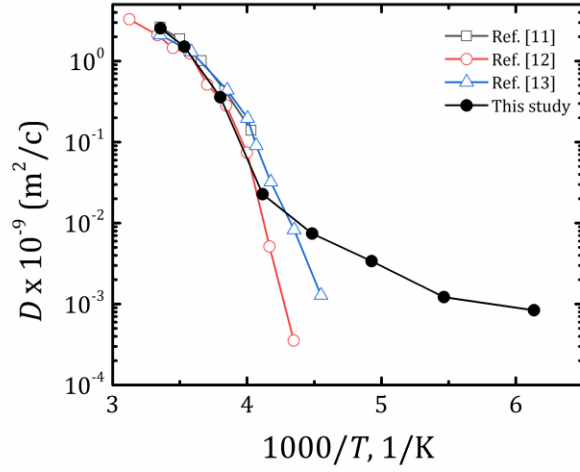


Fig. S4. Temperature dependence of self-diffusion coefficient for bulk TIP5P water. Fild circles correspond to the present study, open simbols are data from Refs. [11–13]

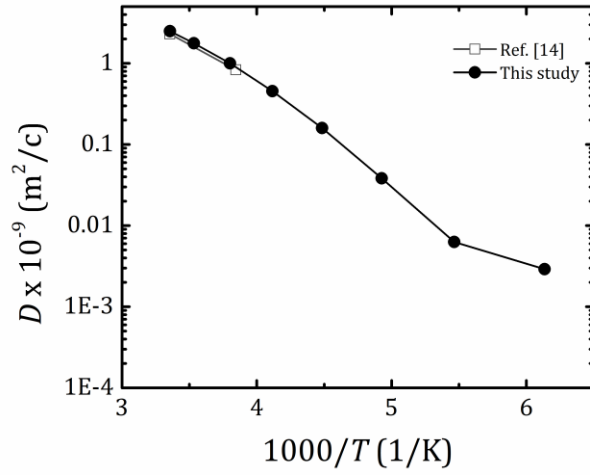
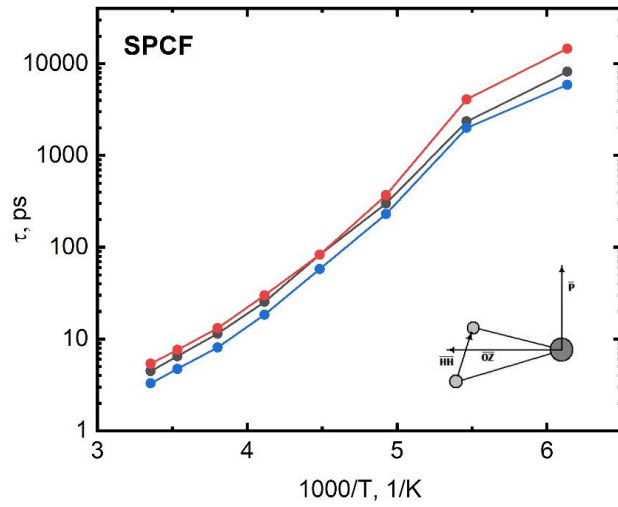


Fig. S5. Fild circles correspond to the present study, open squares are data from Ref. [14].



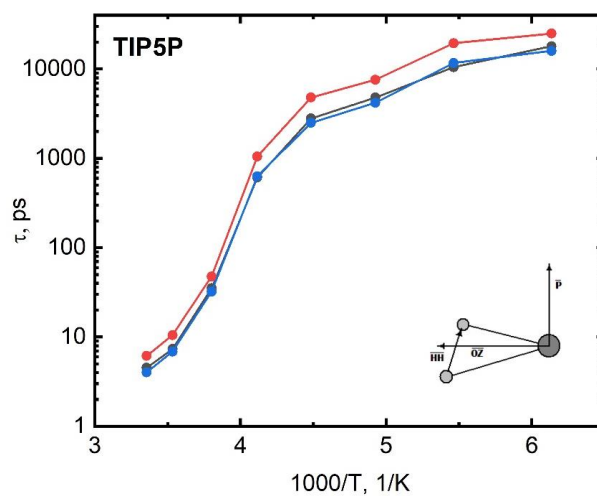
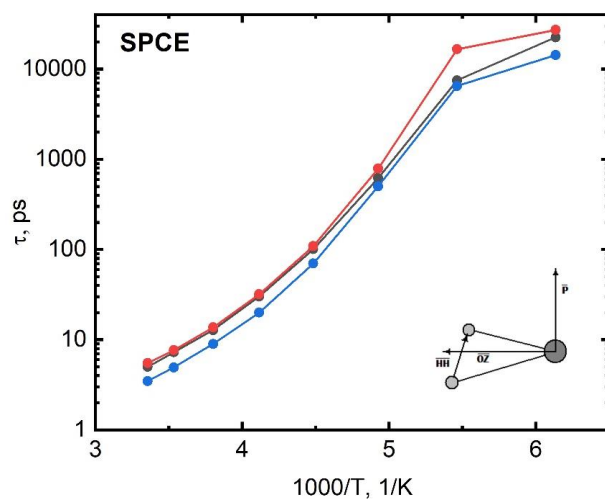
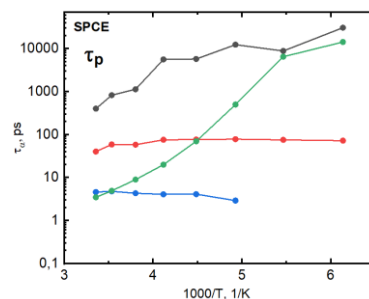
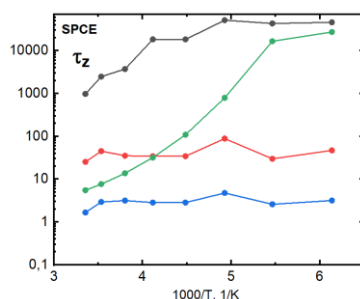
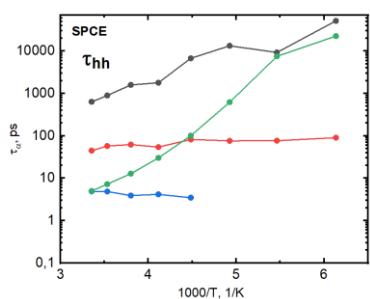


Fig. S6. Temperature dependence of water reorientation correlation times for three molecular directions: HH – vector connecting H atoms, Z – molecular dipole, and P – vector-perpendicular to the plane of the molecule.



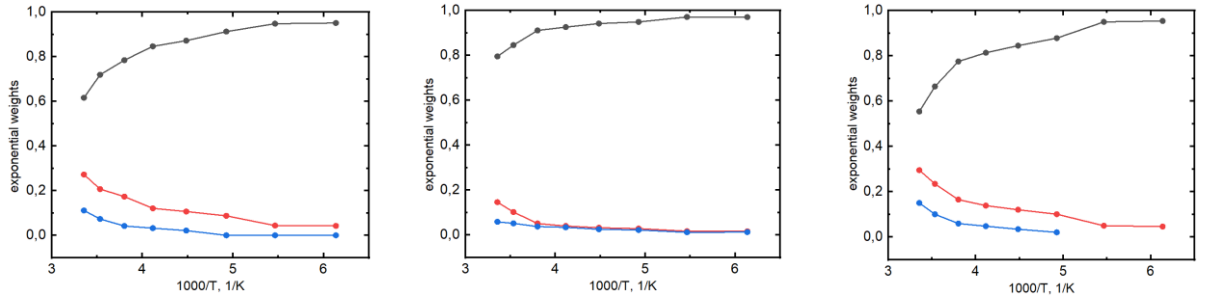


Fig. 5S. Temperature dependence of water reorientation correlation times for three molecular directions: HH – vector connecting H atoms, Z – molecular dipole, and P – vector-perpendicular to the plane of the molecule (upper panels), and corresponding exponential weights (low panels). SPCe water model, corresponding data for bulk system are shown by green line.

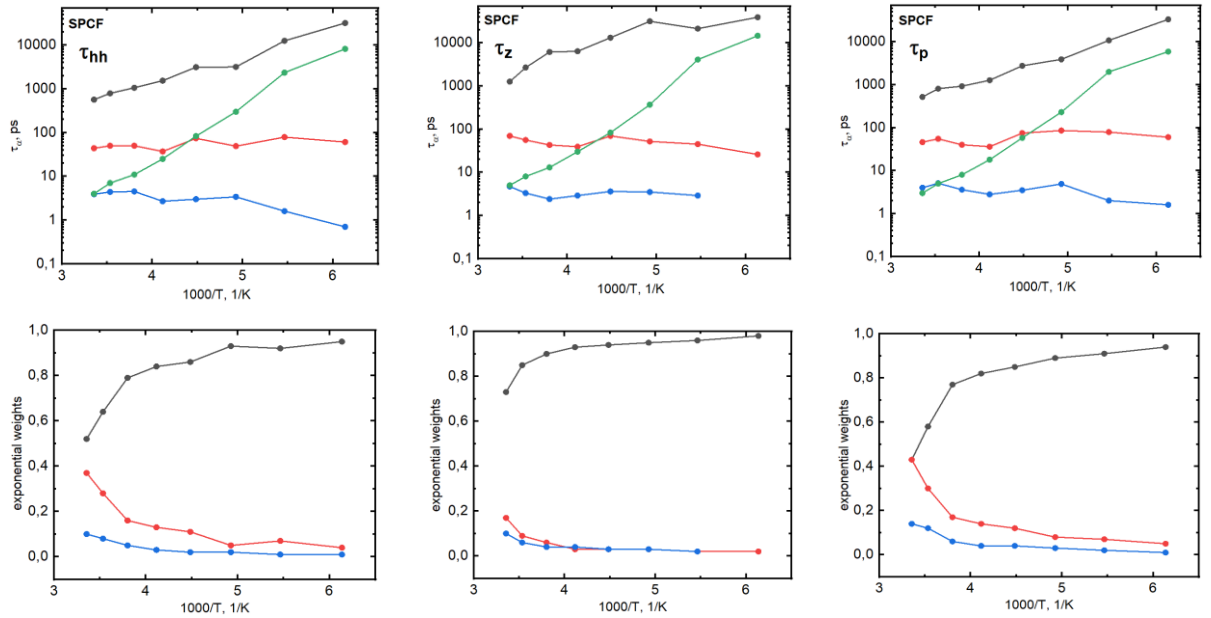
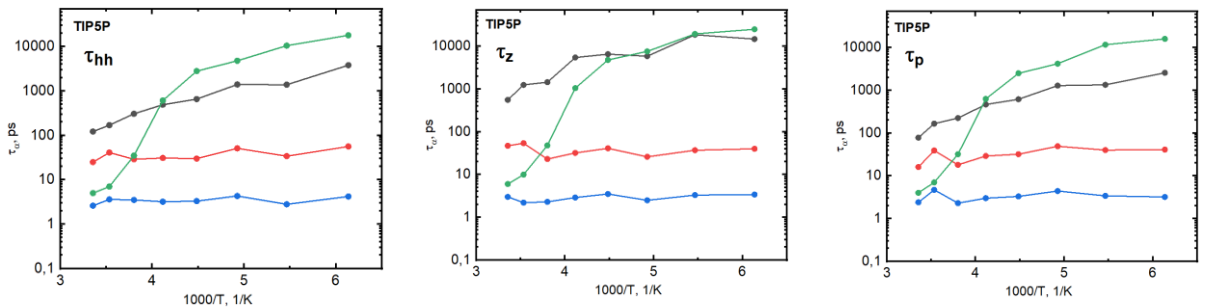


Fig. 8S. Temperature dependence of water reorientation correlation times for three molecular directions: HH – vector connecting H atoms, Z – molecular dipole, and P – vector-perpendicular to the plane of the molecule (upper panels), and corresponding exponential weights (low panels). SPCF water model, corresponding data for bulk system are shown by green line.



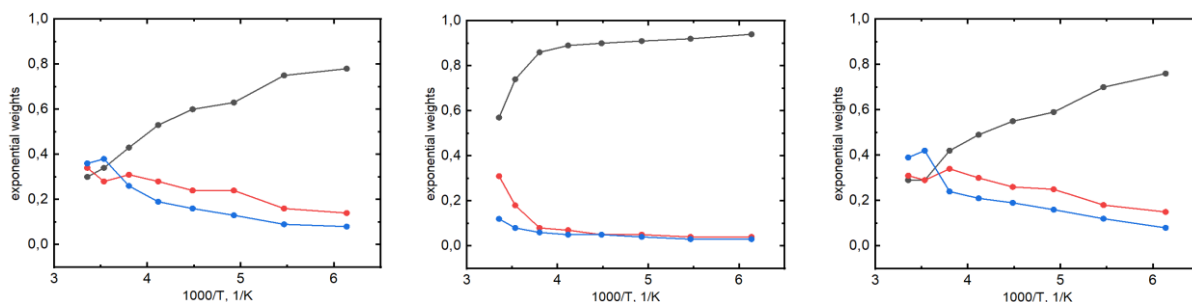


Fig. 9S. Temperature dependence of water reorientation correlation times for three molecular directions: HH – vector connecting H atoms, Z – molecular dipole, and P – vector-perpendicular to the plane of the molecule (upper panels), and corresponding exponential weights (low panels). TIP5P water model, corresponding data for bulk system are shown by green line.

References

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