Electronic Supplementary Material (ESI) for RSC Advances.

Hydrogen bonding of water confined in zeolites and their Zeolitic Imidazolate Framework counterparts

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Electronic Supporting Information

Fig. S1 Zeolite and ZIF forms of FAU topology.

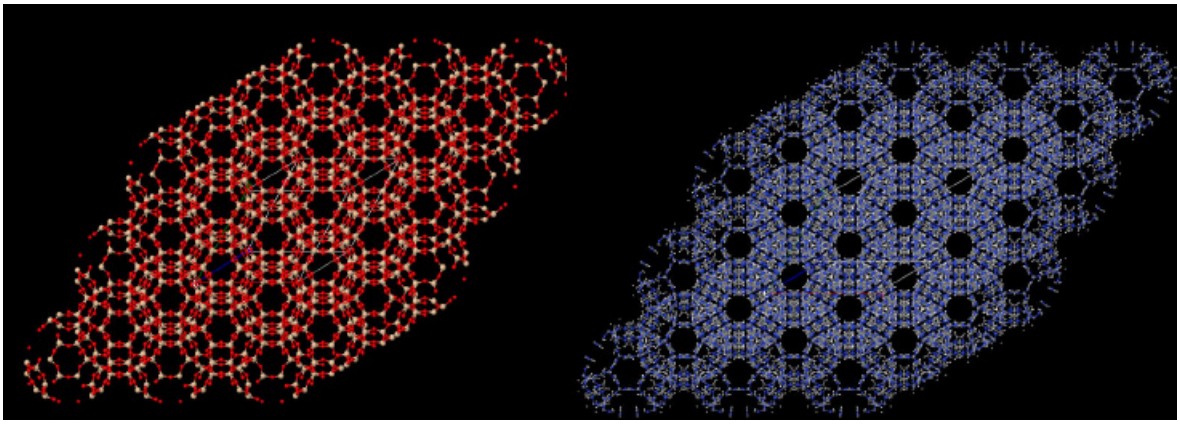

Fig. S2 Zeolite and ZIF forms of FER topology.

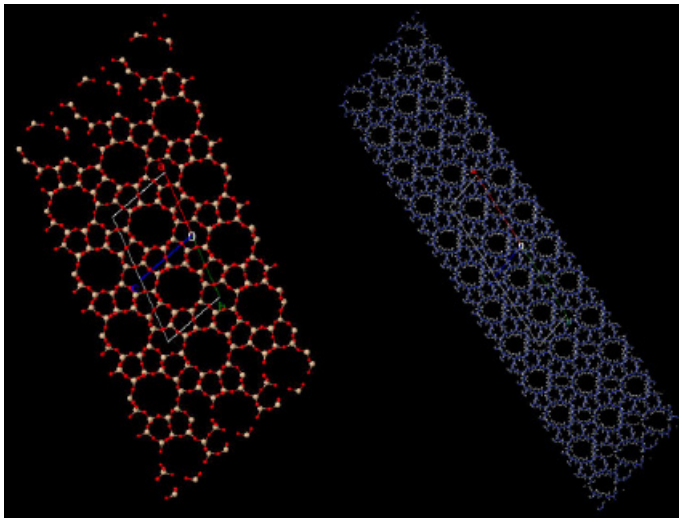

Fig. S3 Zeolite and ZIF forms of MFI topology.

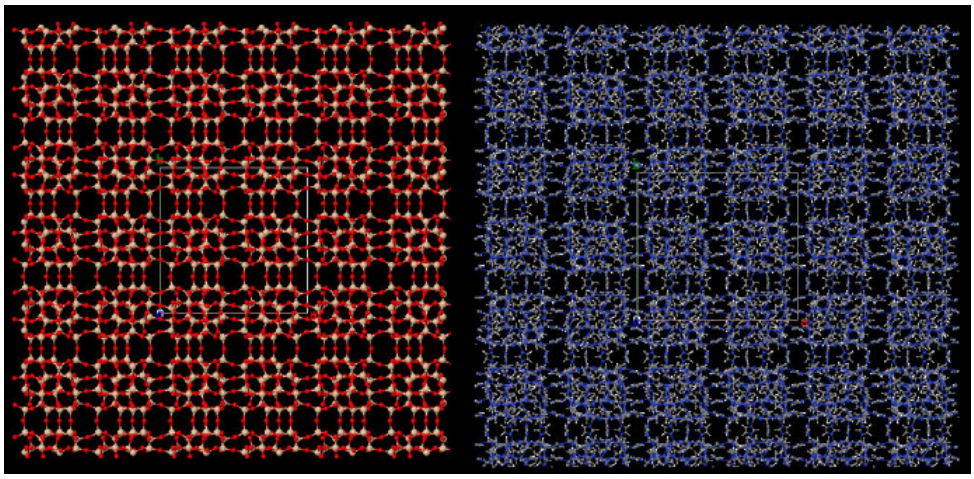

Fig. S4 Zeolite and ZIF forms of RHO topology.

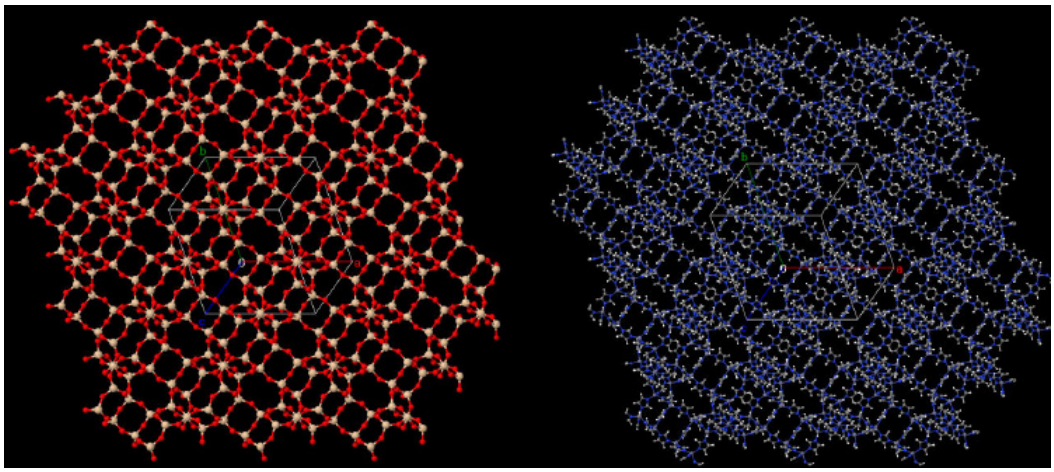

Fig. S5 Geometry and force field parameters of the water molecule for the TIP5P/Ew model.[66]

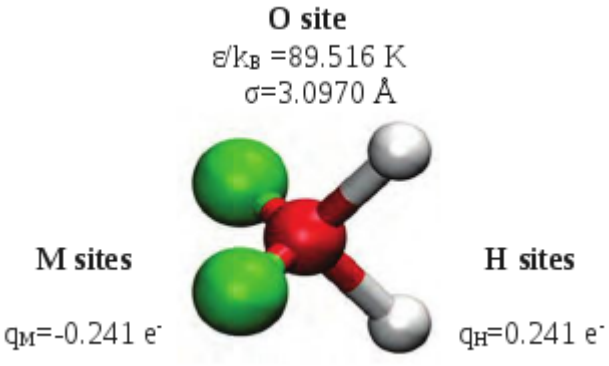

Fig. S6 Pore Size Distributions of the considered structures.

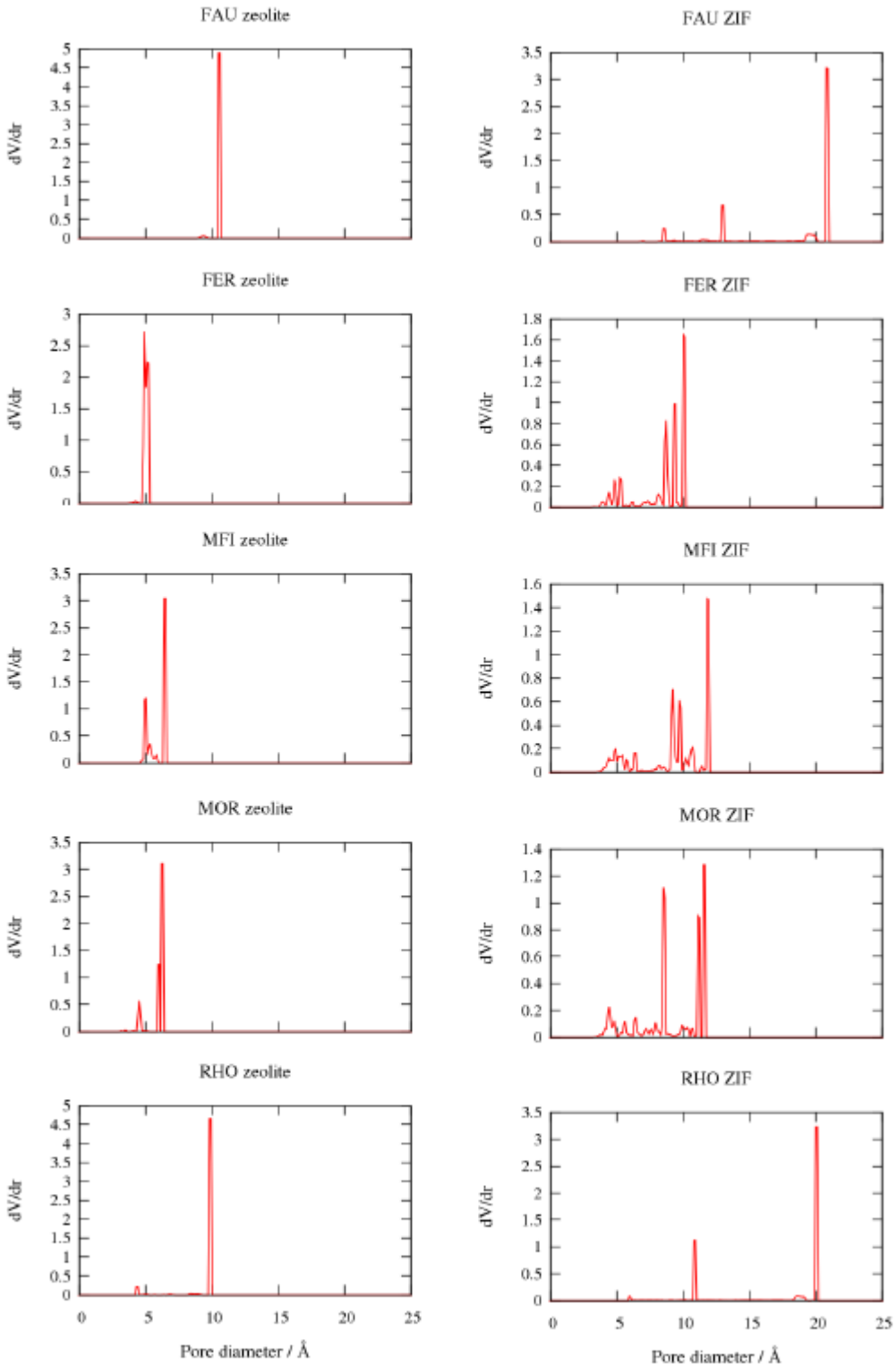

Fig. S7 (a) O-O and (b) O-H Radial Distribution Functions of bulk water at 298.15 K and various values of fugacity.

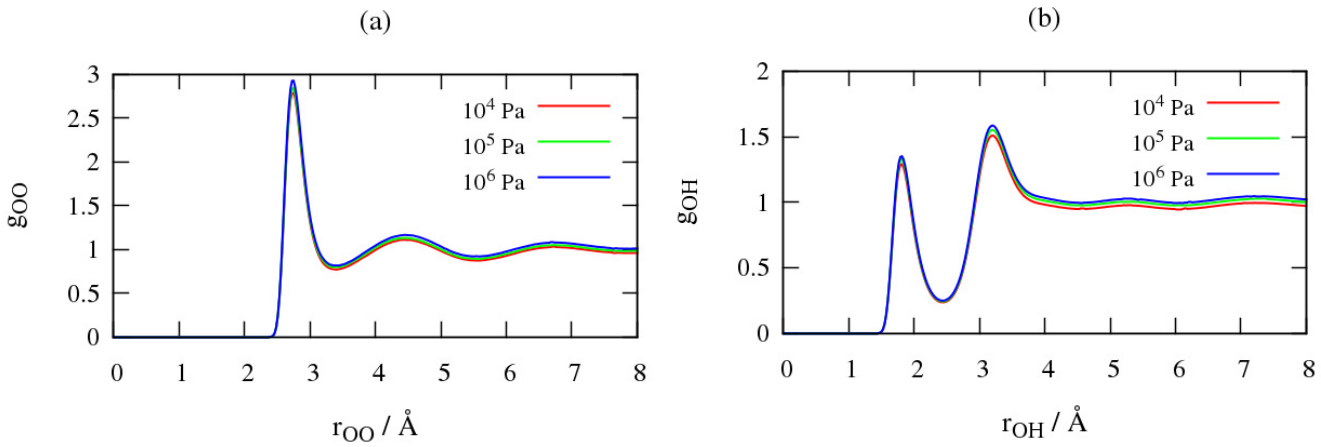

Fig. S8 O-O Radial Distribution Function of water in (a) the zeolites and (b) their ZIF counterparts at 298.15 K for 1 MPa (red), 10MPa (green) and 100 MPa (blue).

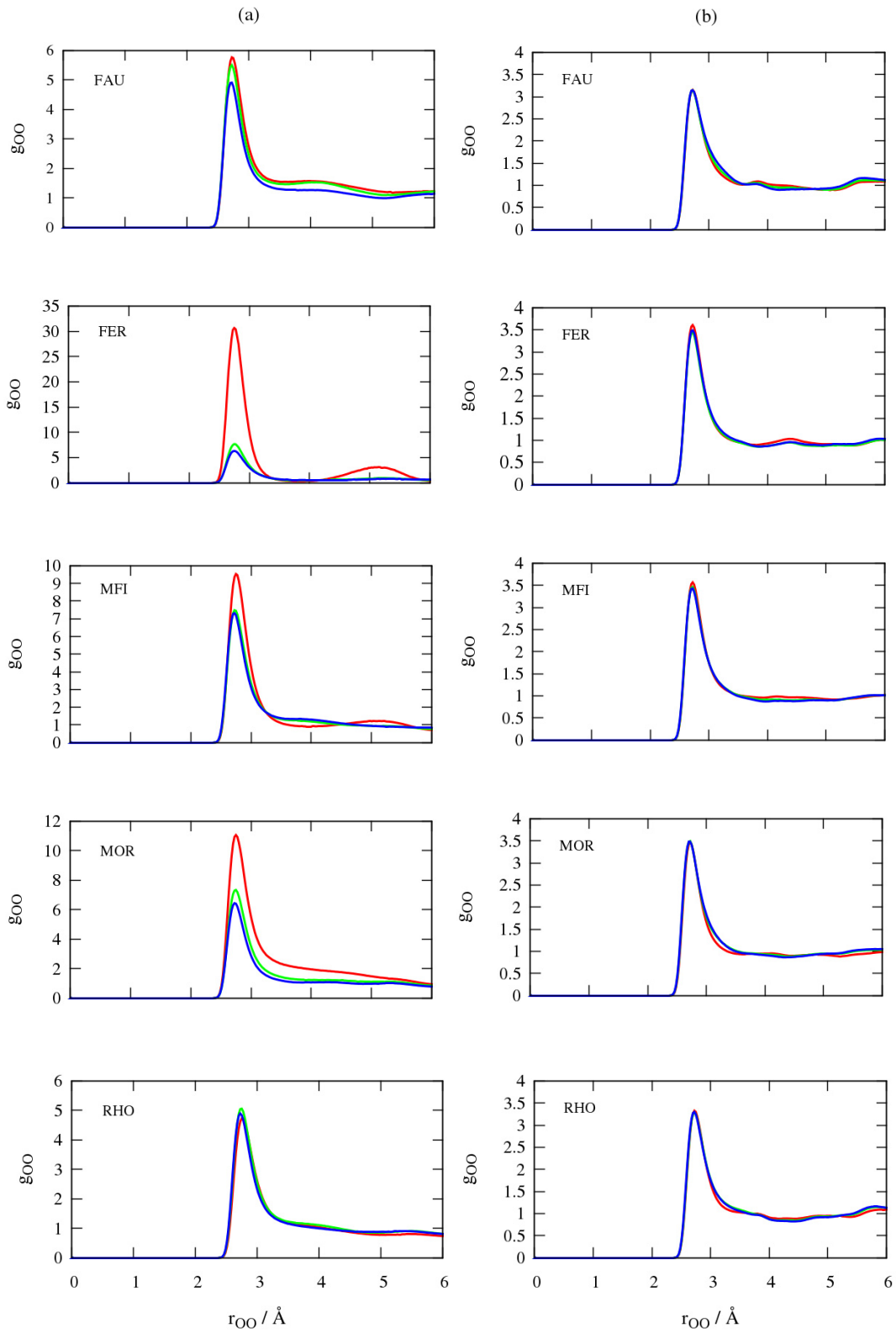

Fig. S9 O-H Radial Distribution Function of water in (a) the zeolites and (b) their ZIF counterparts at 298.15 K for 1 MPa (red), 10MPa (green) and 100 MPa (blue).

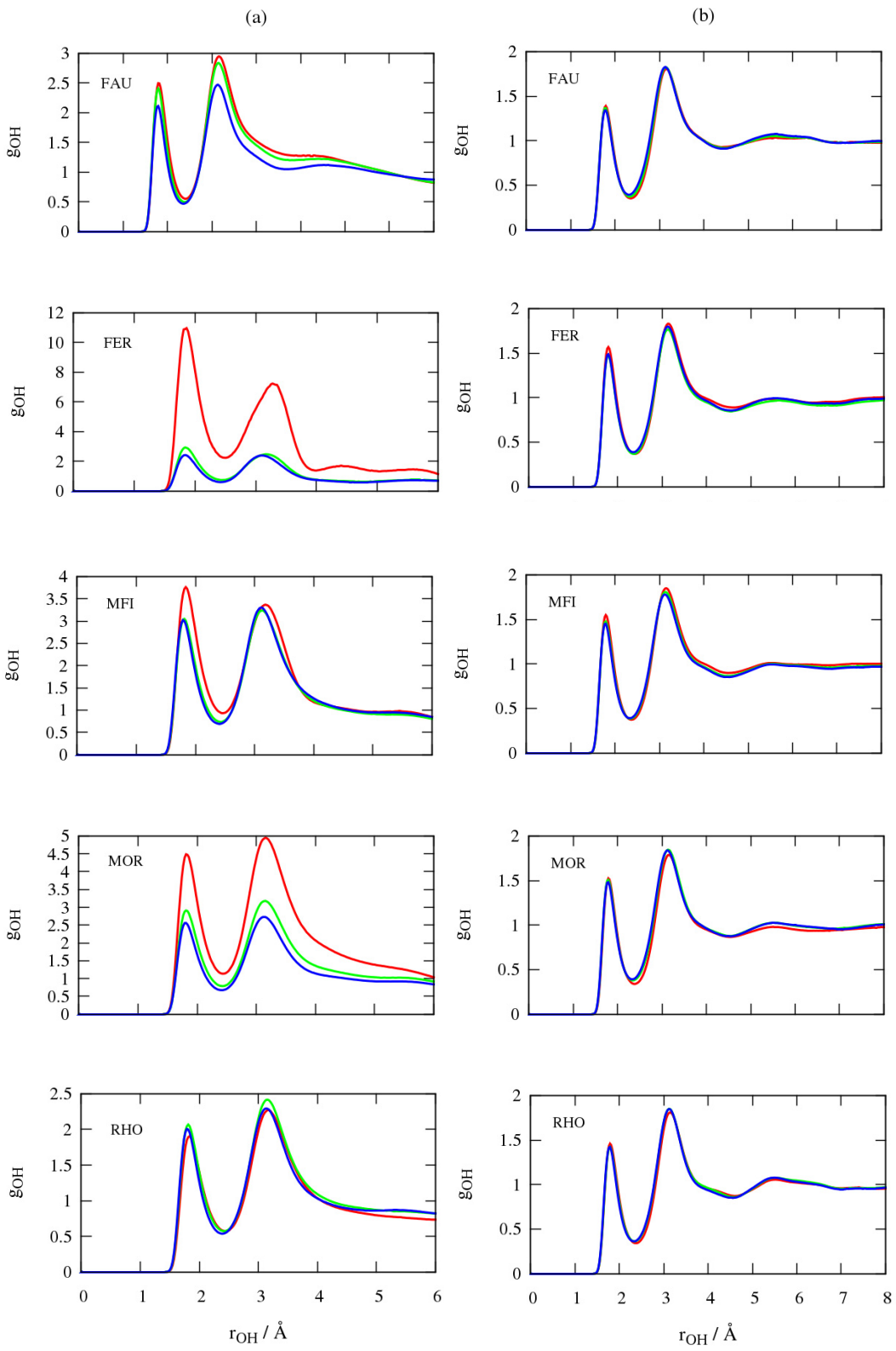

Fig. S10 Cluster size distribution for water in the highly hydrated structures.