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Supplementary material to:

Simulation of Calcium Phosphate Species in Aqueous
Solution: Force Field Derivation

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Figure S1: H_2PO_4^- -water pair distribution functions. *Ab initio* data (run for a few tens of ps) are shown with a dashed red line, force field data (run for about 1 ns) with a full green line. Atom labels as in the main manuscript; d is the distance in Å, P the probability. Note that these PDFs have been considered only as a rough guide to initial force field fitting.

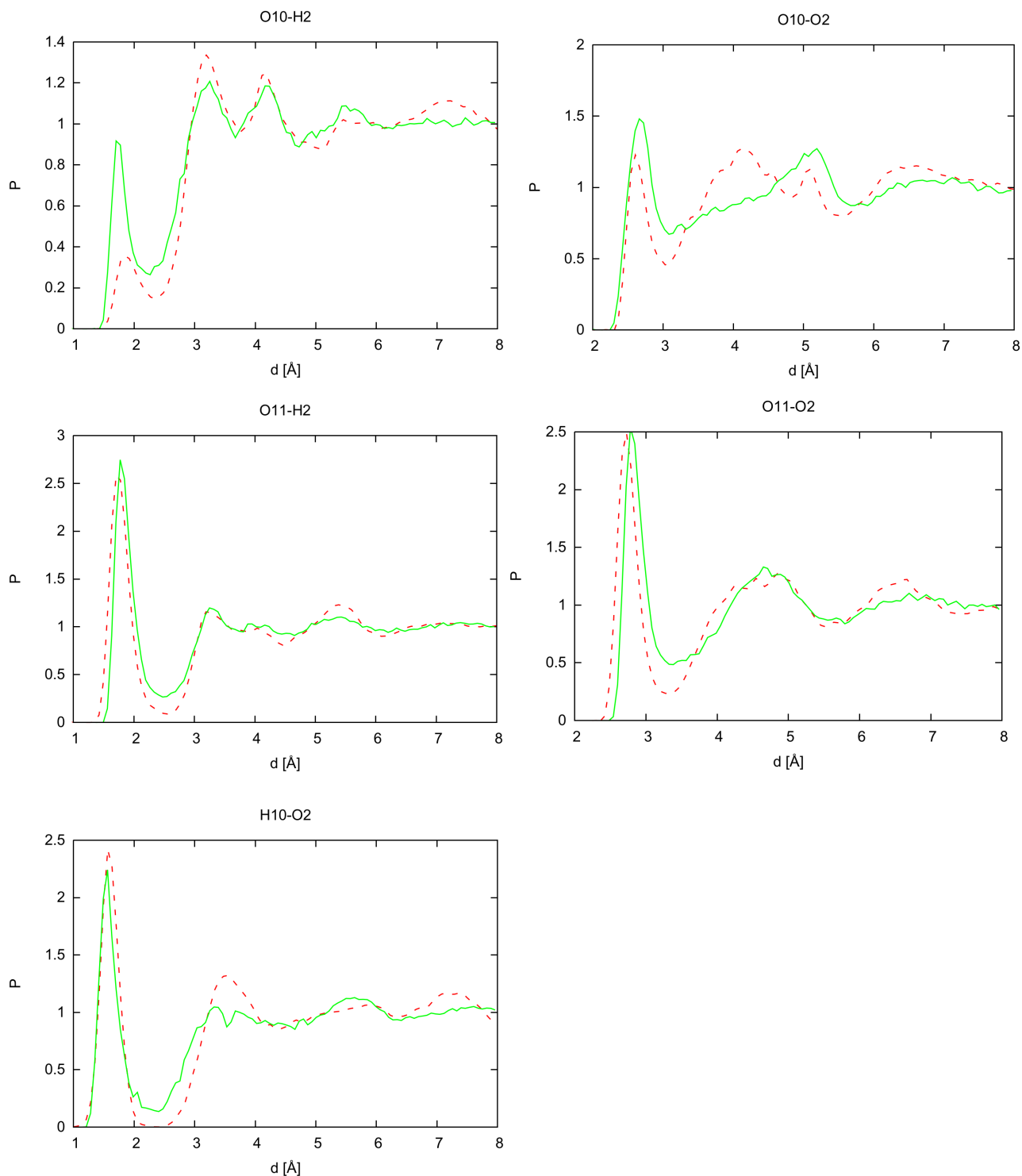


Figure S2: HPO_4^{2-} -water pair distribution functions. Colors and labels as in Figure S1.

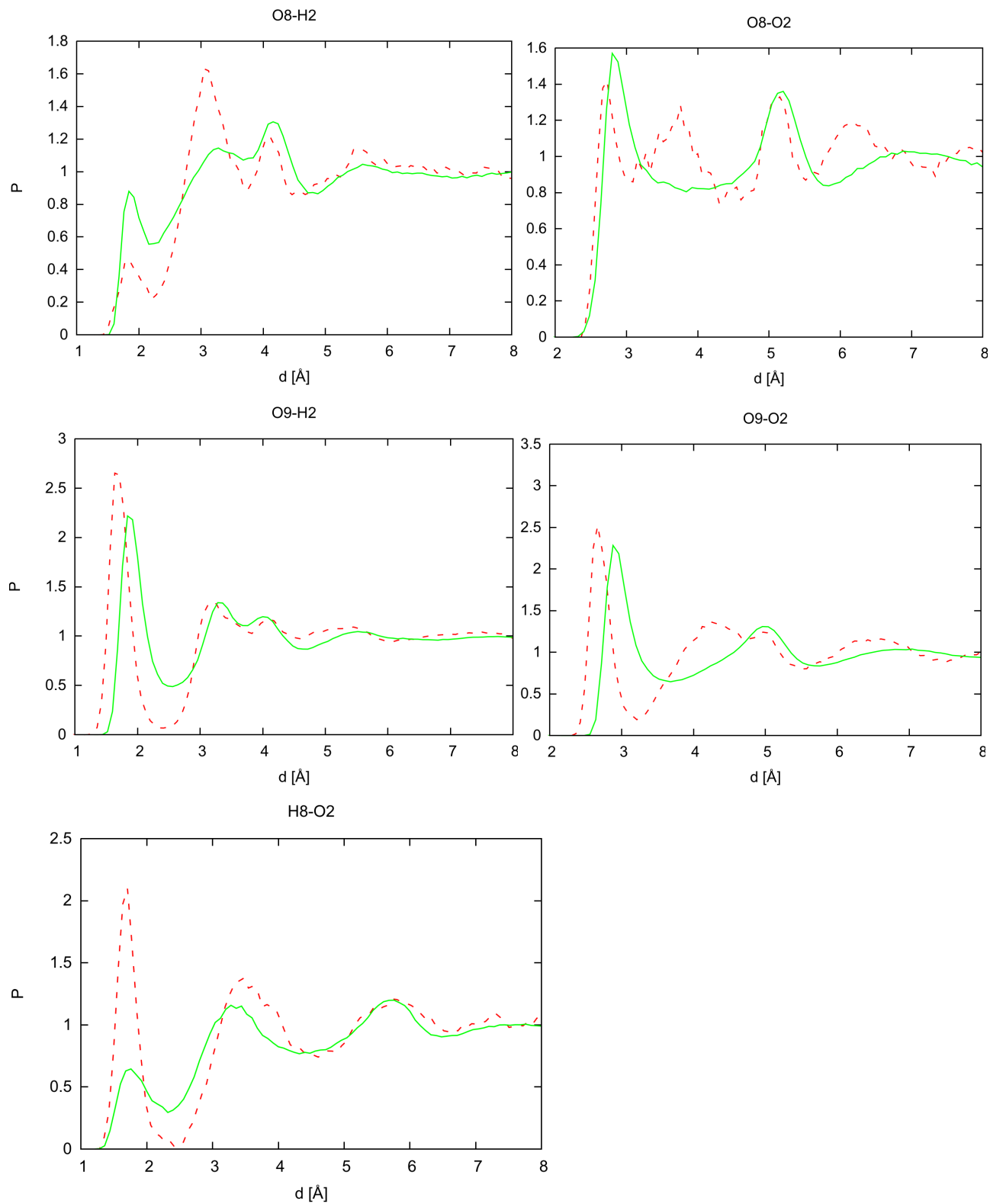


Figure S3: PO₄²⁻-water pair distribution functions. Colors and labels as in Figure S1.

