Article:
Demichelis, R. orcid.org/0000-0001-9741-213X, Garcia, N.A., Raiteri, P. orcid.org/0000-0003-0692-0505 et al. (4 more authors) (2018) Simulation of calcium phosphate species in aqueous solution: force field derivation. Journal of Physical Chemistry B, 122 (4). pp. 1471-1483. ISSN 1520-6106

https://doi.org/10.1021/acs.jpcb.7b10697

Supplementary material to:

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

Raffaella Demichelis,[1] Natalya A. Garcia,[1] Paolo Raiteri,[1] Riccardo Innocenti Malini,[2,3] Colin L. Freeman,[2] John H. Harding[2] and Julian D. Gale[1]*

[1] Curtin Institute for Computation, The Institute for Geoscience Research (TIGeR) and Department of Chemistry, Curtin University, PO Box U1987, Perth, WA 6845, Australia.

[2] Department of Materials Science and Engineering, University of Sheffield, Sheffield, S1 3JD, United Kingdom.

[3] Laboratory for Biomimetic Membranes and Textiles, Empa, Swiss Federal Laboratories for Materials Science Technology, St. Gallen 9014, Switzerland.

*raffaella.demichelis@curtin.edu.au

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.

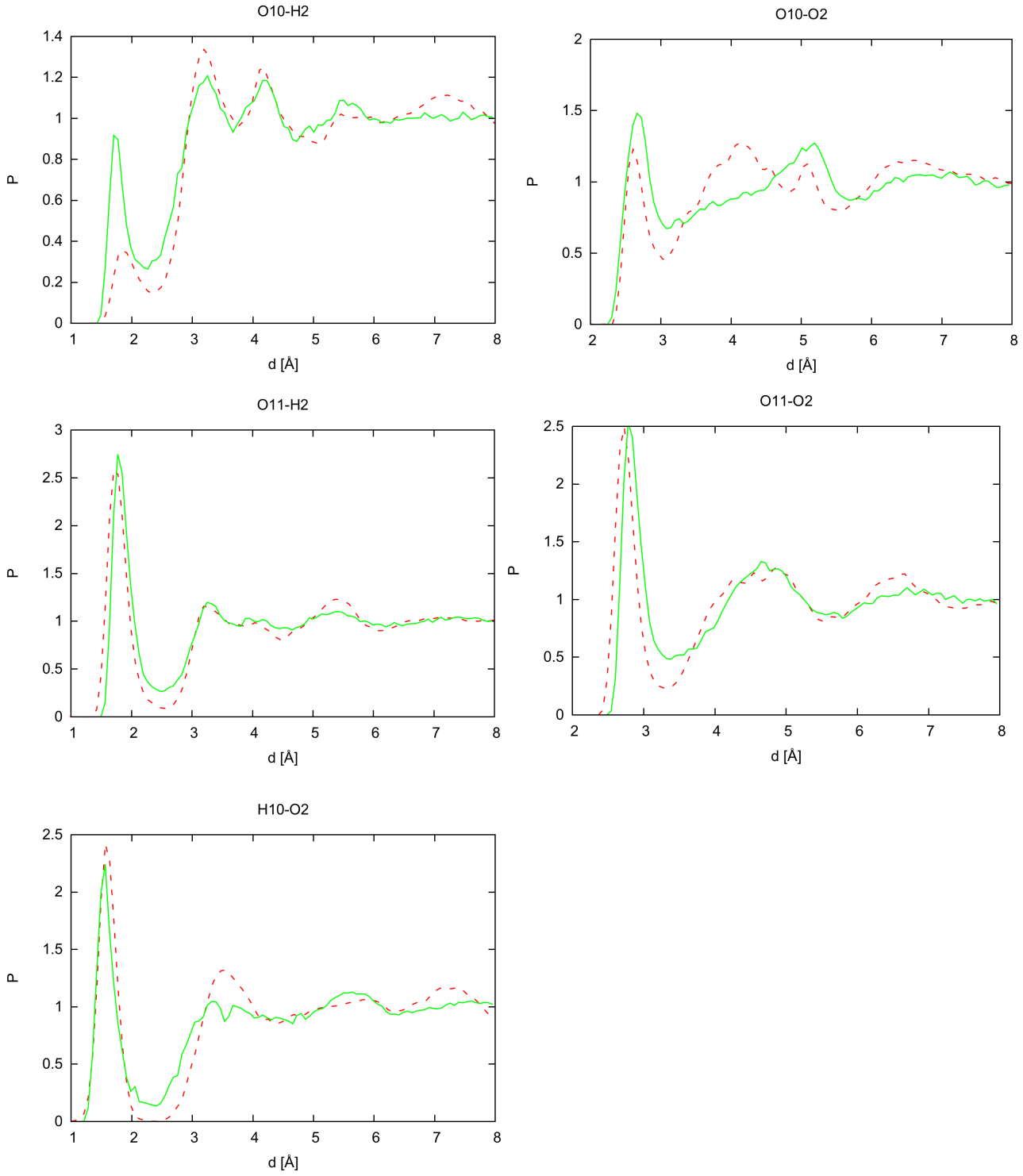

Figure S2: HPO_4^{2-}-water pair distribution functions. Colors and labels as in Figure S1.

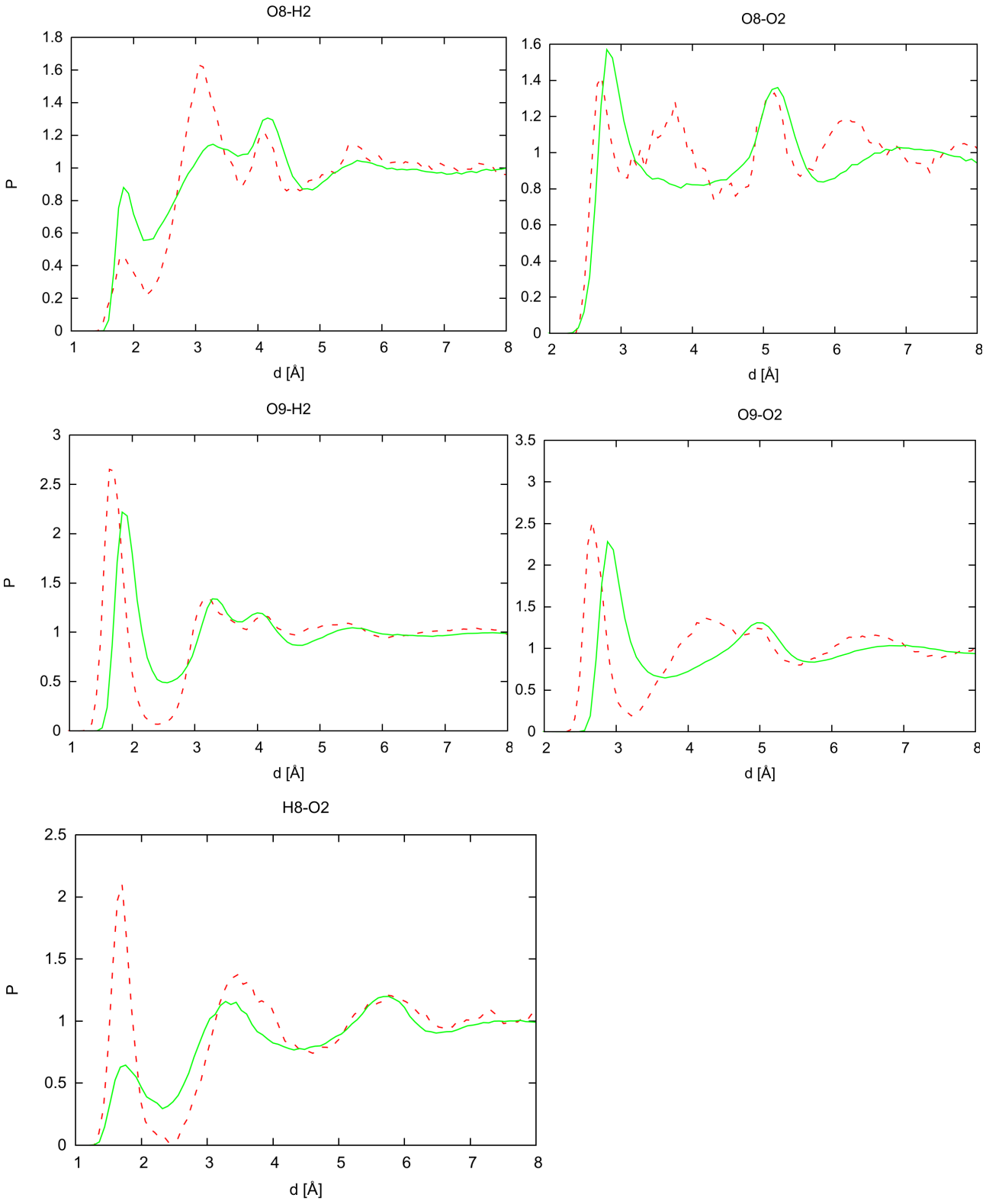

Figure S3: PO_4^{2-}-water pair distribution functions. Colors and labels as in Figure S1.