Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supporting Information

## Insights into the hydrogen bond network topology of phosphoric acid and water systems

Austėja Mikalčiūtė[a] and Linas Vilčiauskas*[a,b]

[a]Institute of Chemistry, Vilnius University, Saulėtekio al. 3, LT-10257, Vilnius, Lithuania.
[b]Center for Physical Sciences and Technology (FTMC), Saulėtekio al. 3, LT-10257, Vilnius, Lithuania.
*E-mail: linas.vilciauskas@chgf.vu.lt

## 1 Force field benchmarks for $H_3PO_4$

### 1.1 Liquid densities

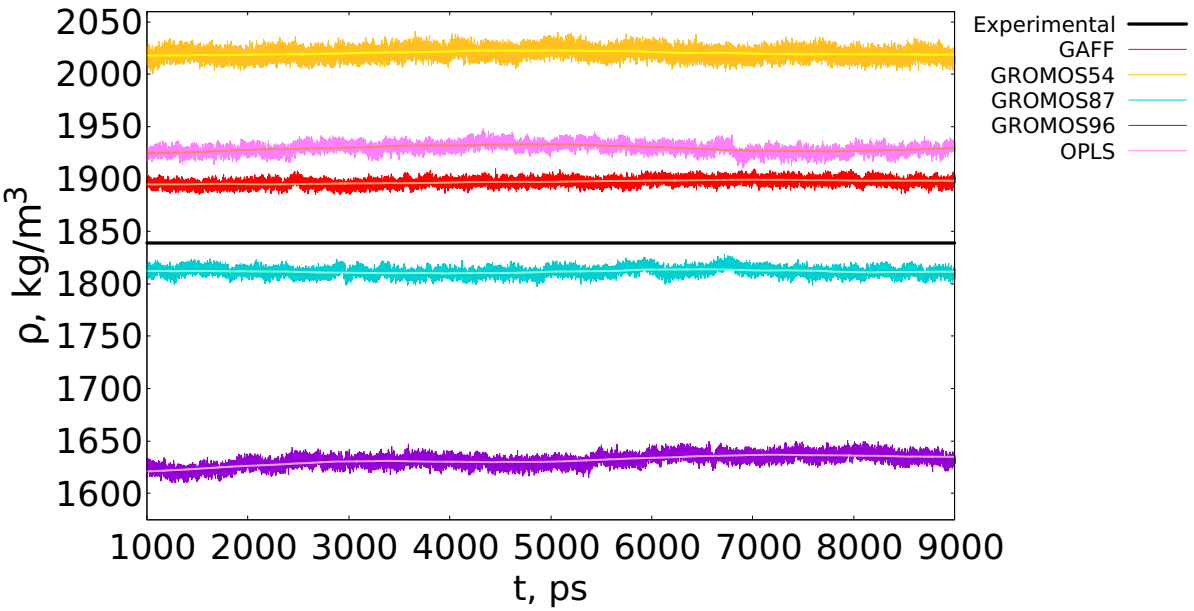


Figure 1: Molecular dynamics simulations of liquid $H_3PO_4$ in NPT ensemble. The experimental density is marked by a black line.

## 1.2 Radial Distribution Functions (RDF)

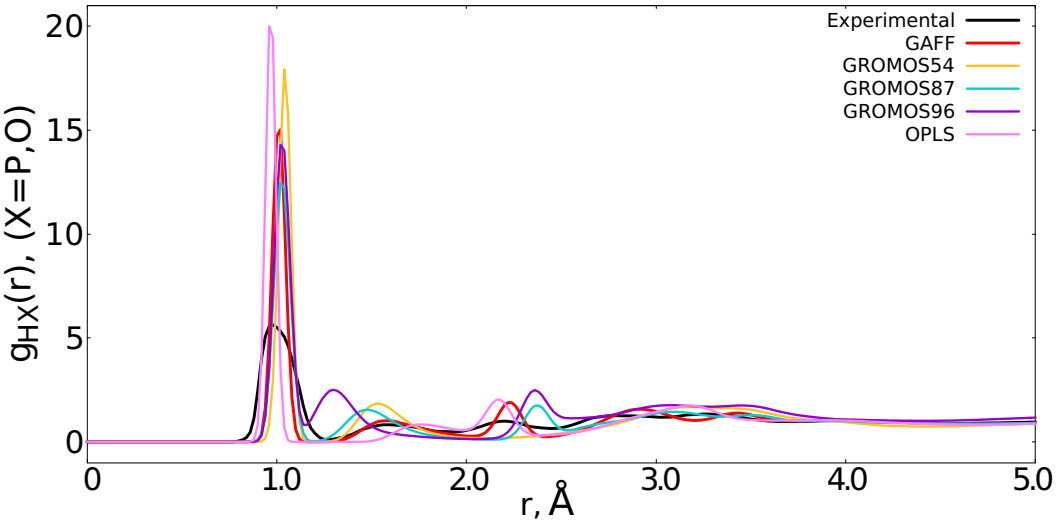


Figure 2: Molecular dynamics simulated $g_{HX}(r), (X = P, O)$ RDFs of liquid $H_3PO_4$ in NPT ensemble.

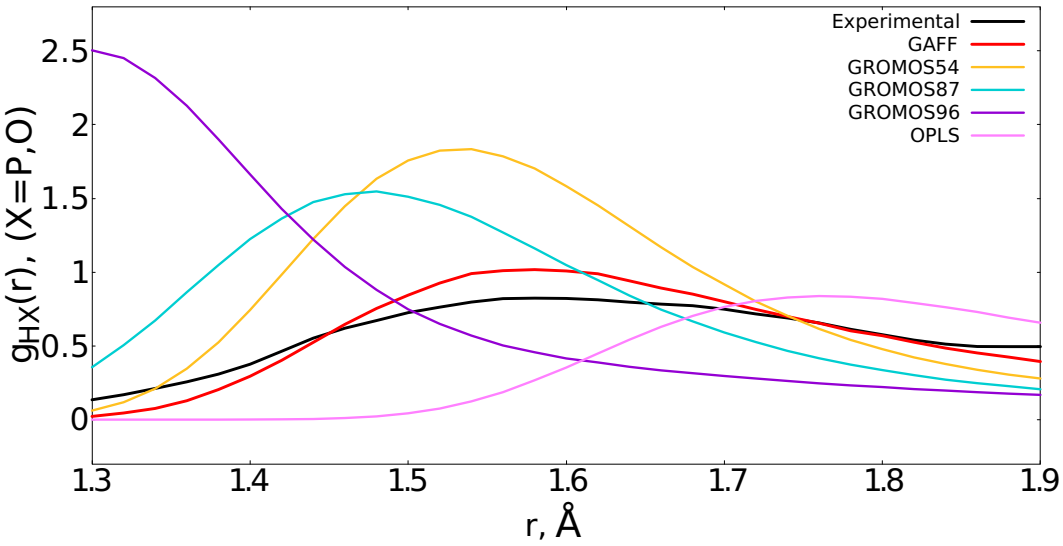


Figure 3: Molecular dynamics simulated $g_{HX}(r), (X = P, O)$ RDFs of liquid $H_3PO_4$ in NPT ensemble. Hydrogen bonding region between 1.3 Åand 1.9 Å.