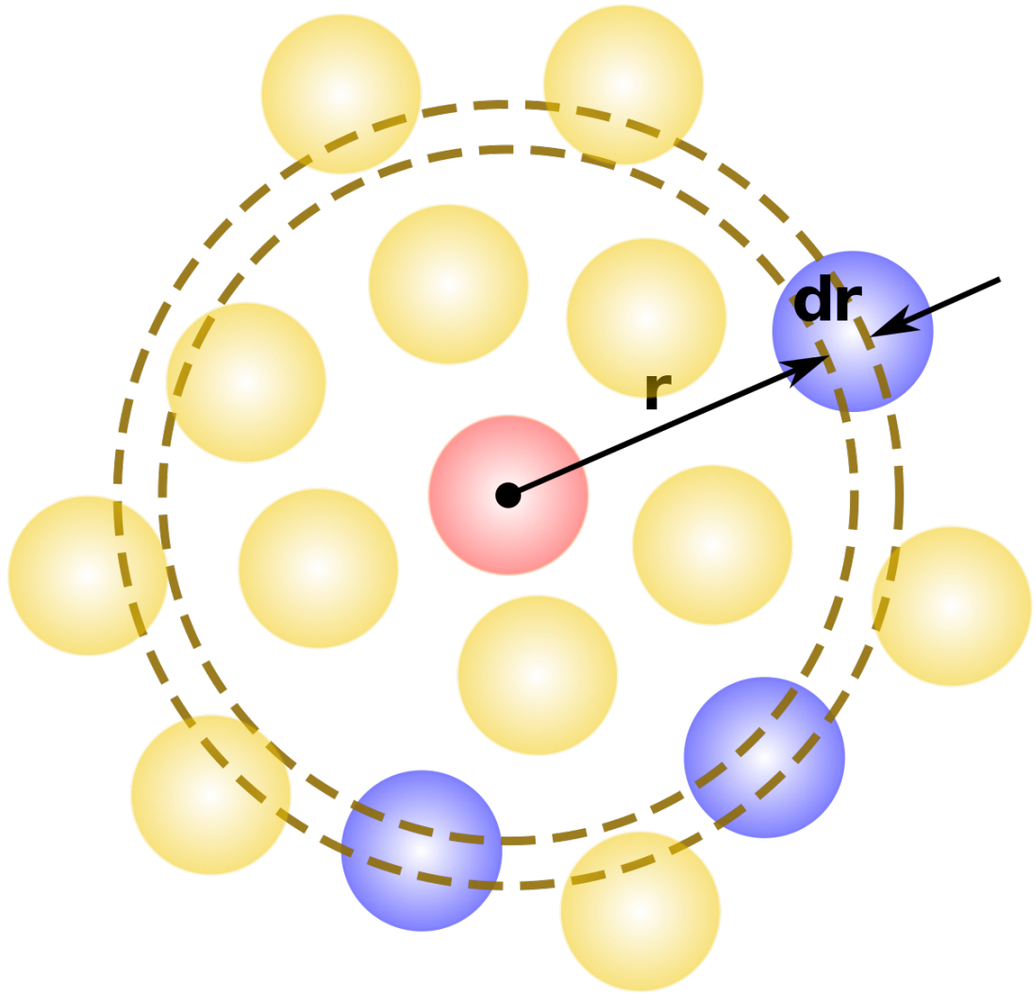
Radial Distribution Function

Radial Distribution Function

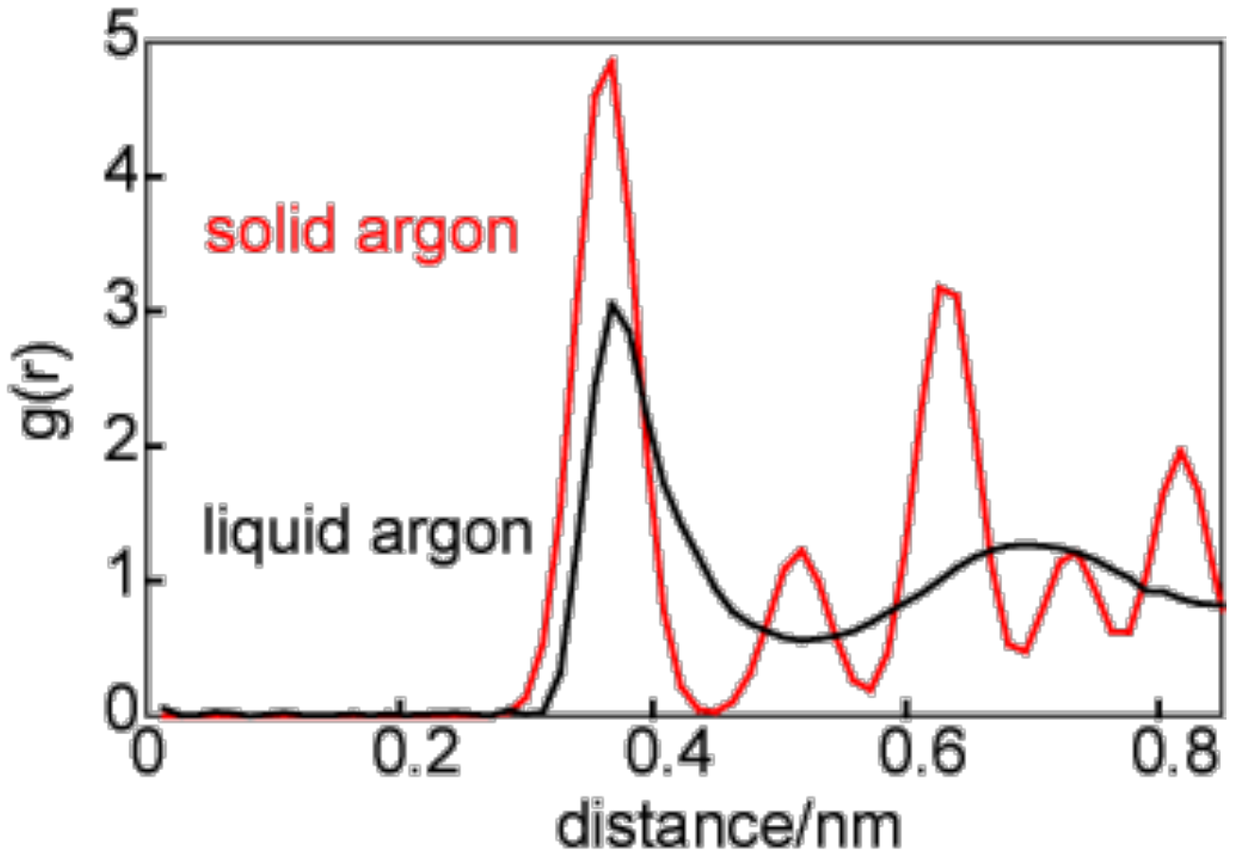


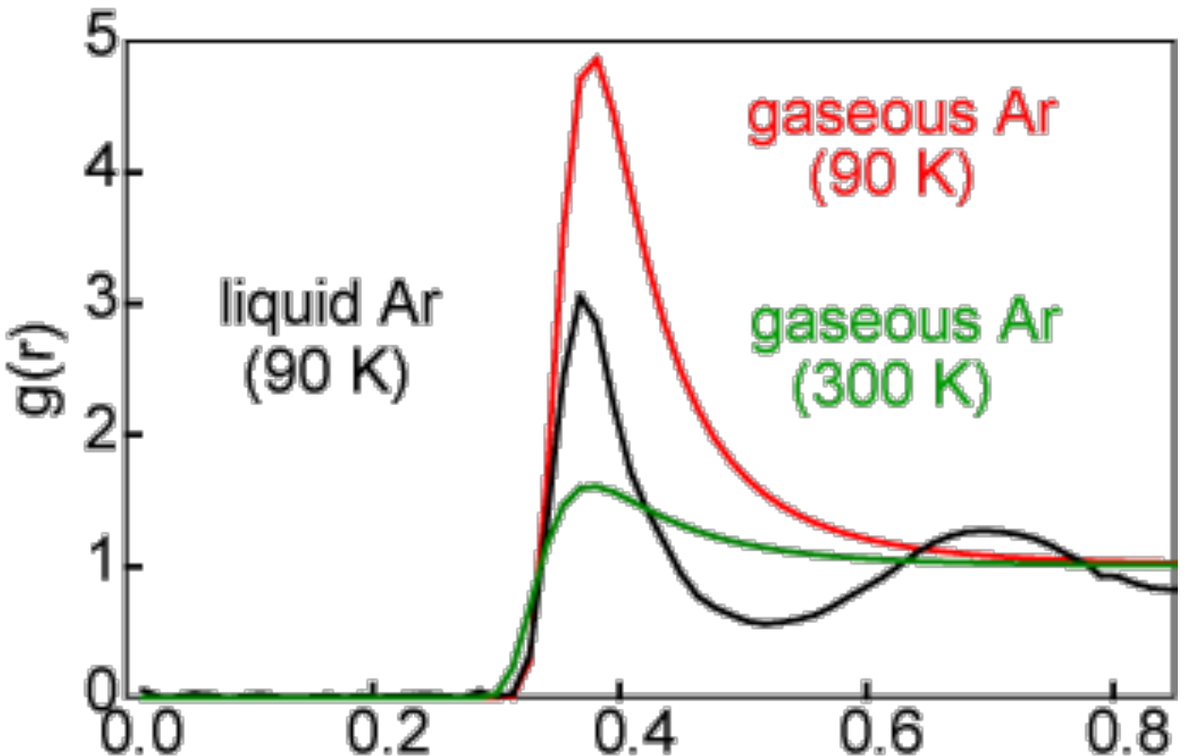
$$g(r) = \frac{\text{No. Of atoms in a shell of radius } r \text{ and thickness } \Delta r}{\rho \times 2\pi r \Delta r}$$

$$g(r) = \frac{\Delta n(r)}{\rho \times 2\pi r \Delta r}$$

Equivalent to radial probability (density) of an atom being at distance r from another atom

Empirically Measured RDF (neutron and x-ray scattering)

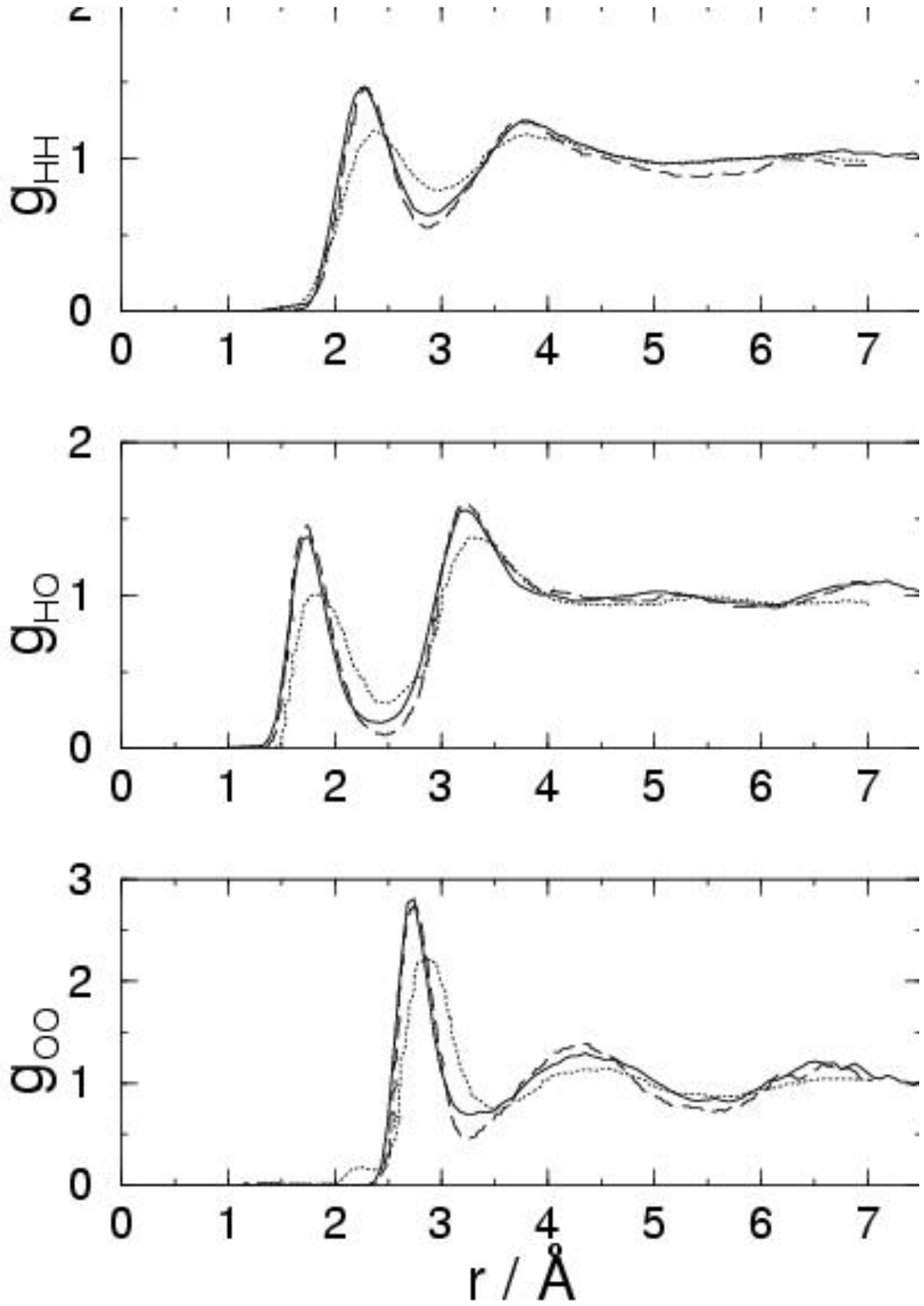




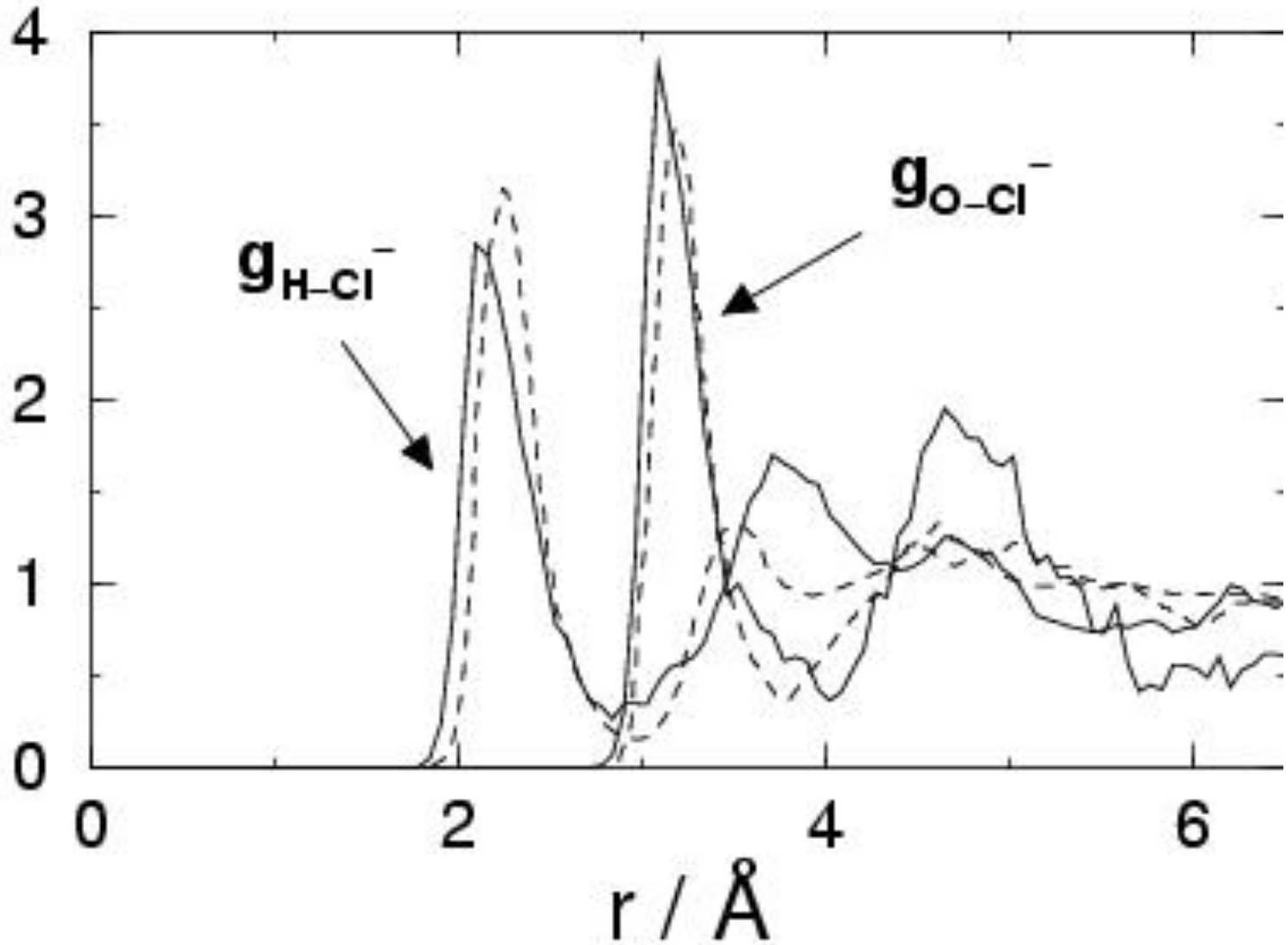
Water

MD Simulation

Neutron Diffraction

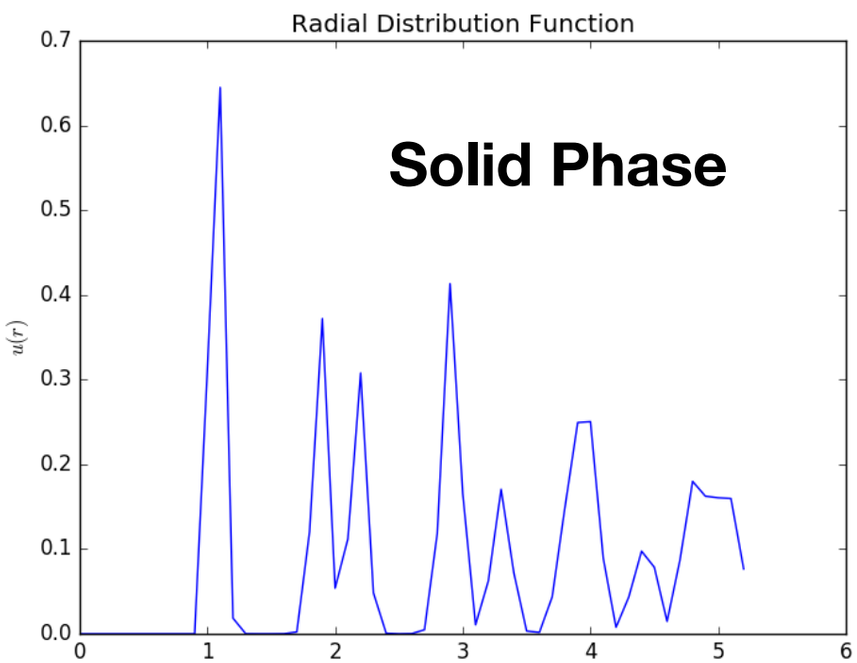


HCl

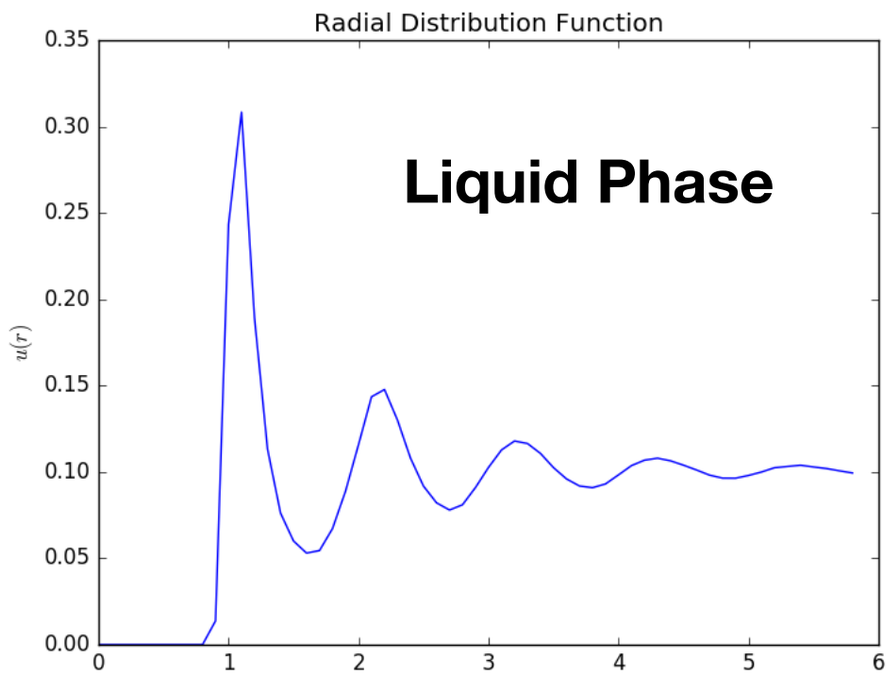


Simulated RDF for 2-D Lennard Jones System

$T = 0.17 \qquad P = 0.4$



$T = 0.6 \qquad P = 0.4$



$T = 2.5 \qquad P = 0.4$