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Materials and Process Simulation Center

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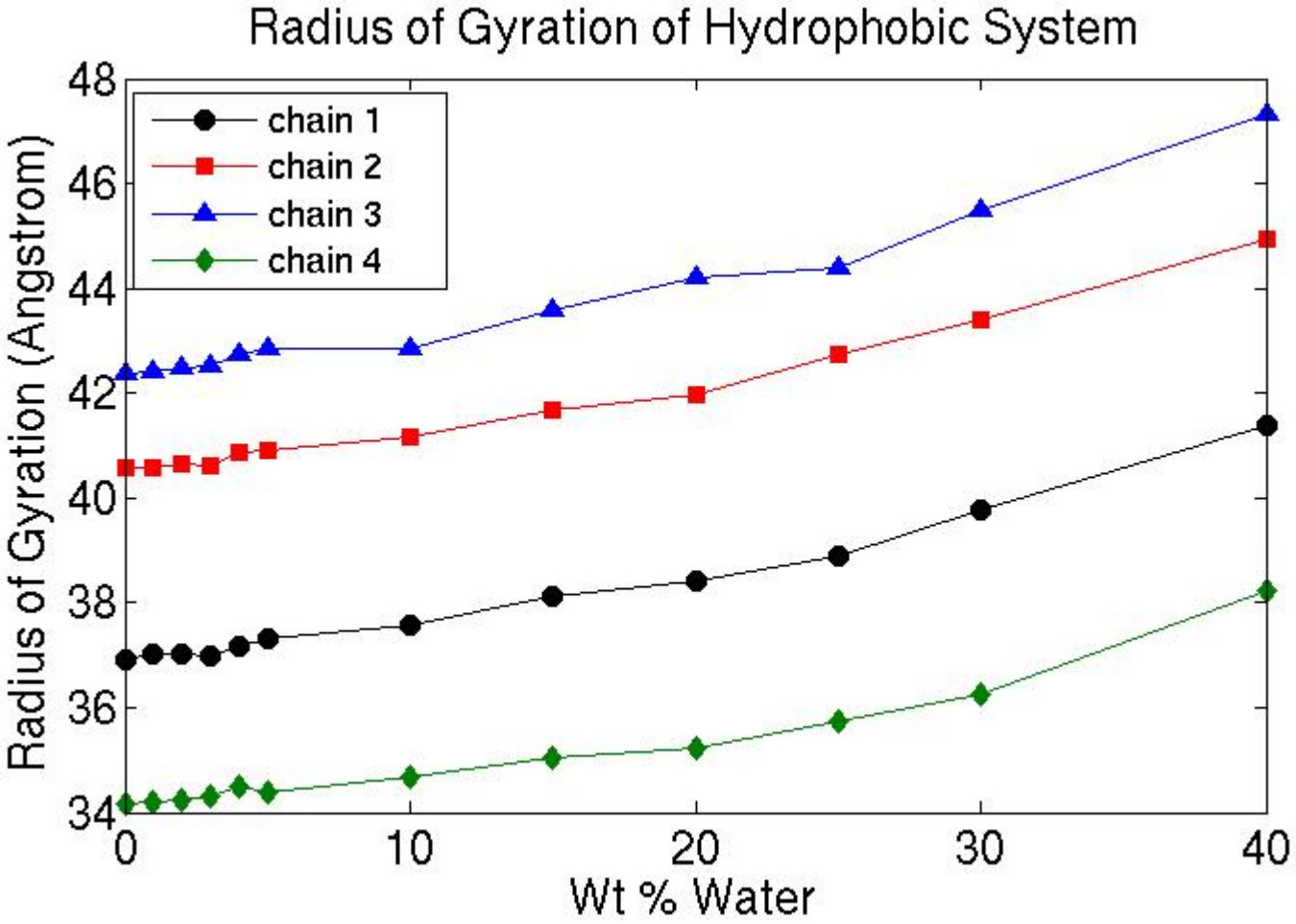
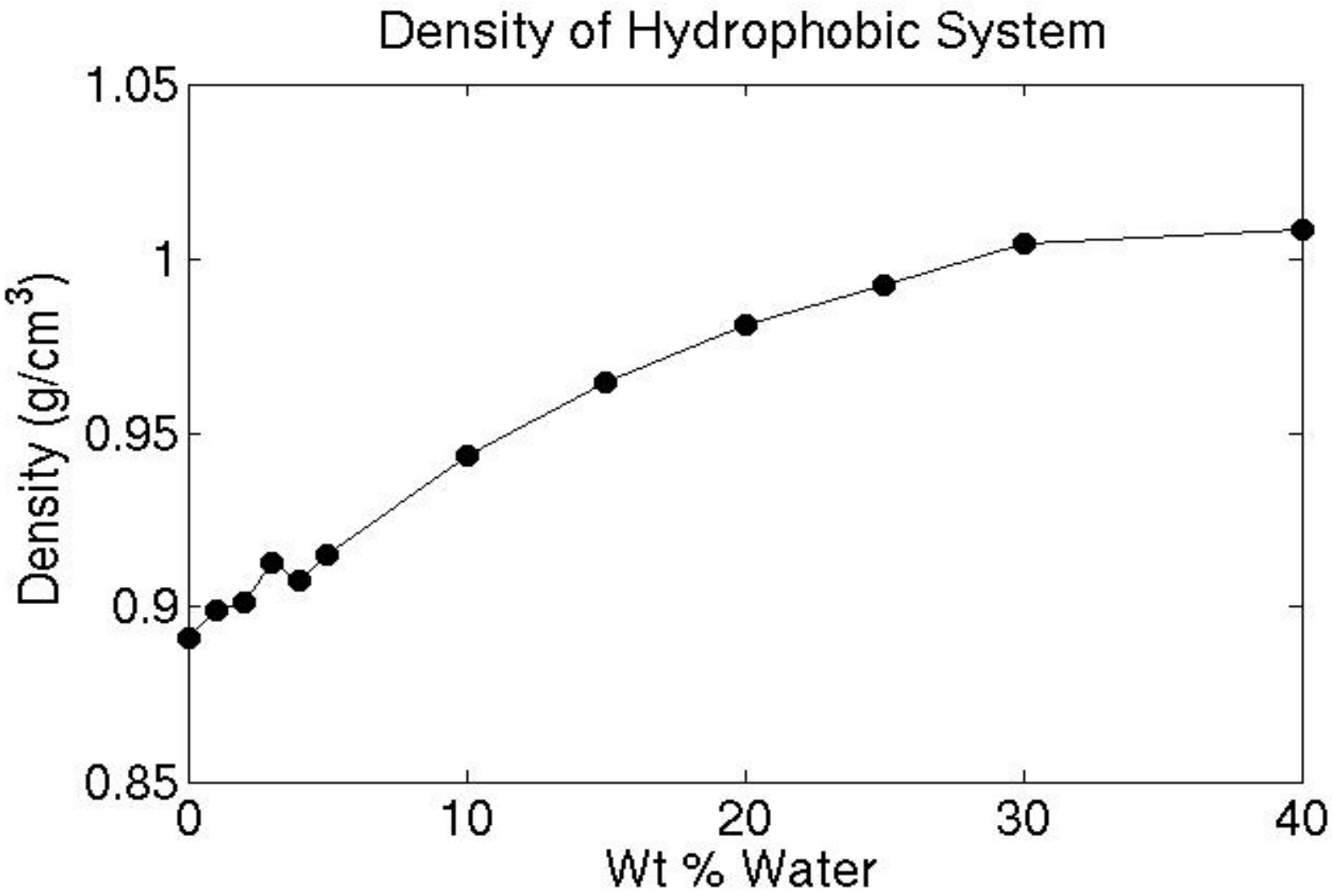
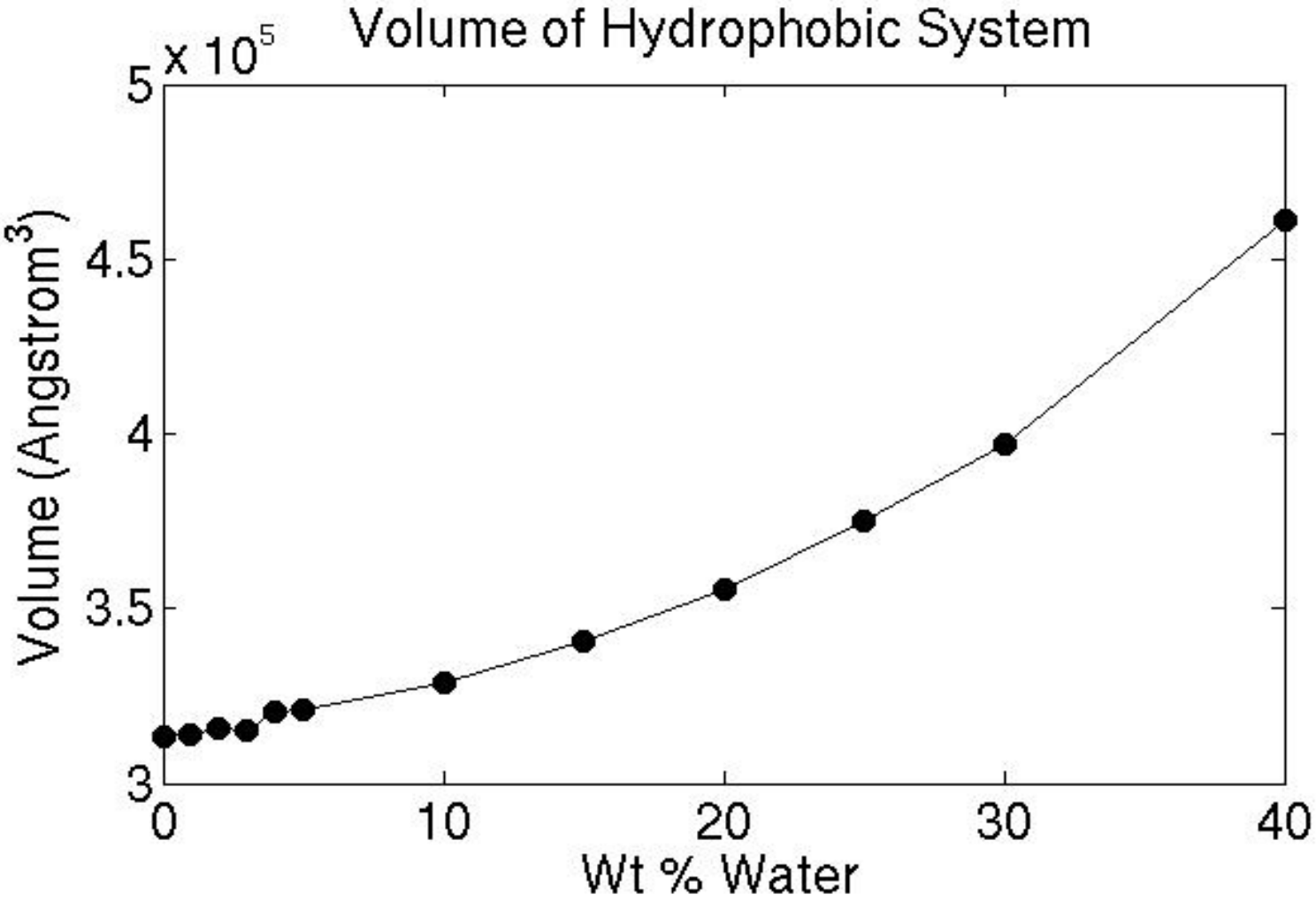
Hydrophobic System - Summary

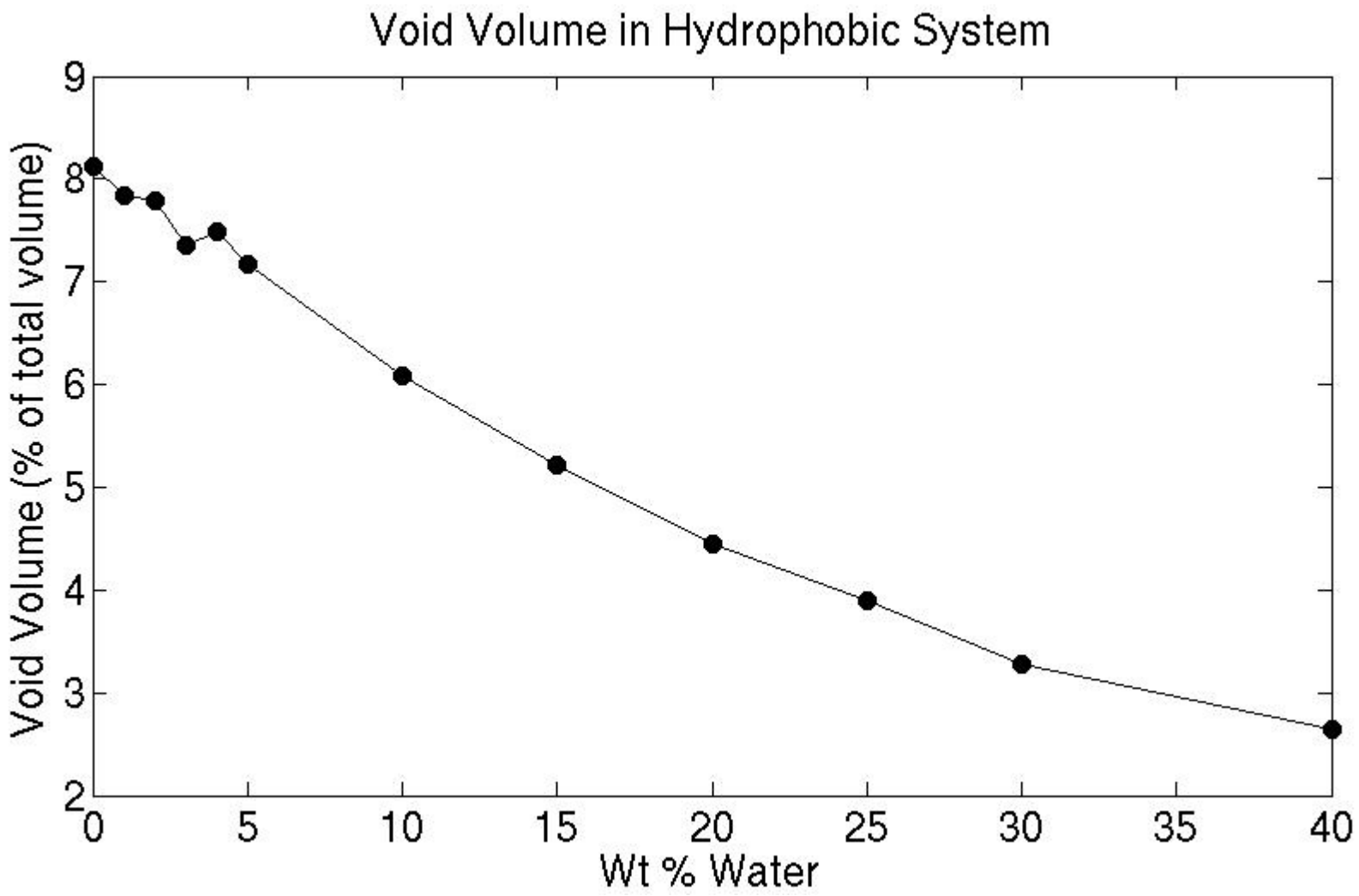
- 10 and 30% structures still running (data points to be added to all plots)
- Densities reasonable (0.9 for dry) with good entanglement
- Densities, volumes, stresses all show kinks at 20%
- Equilibration procedure: CED for dry structure, not for solvated systems. Add waters at random, equilibrate with NPT.



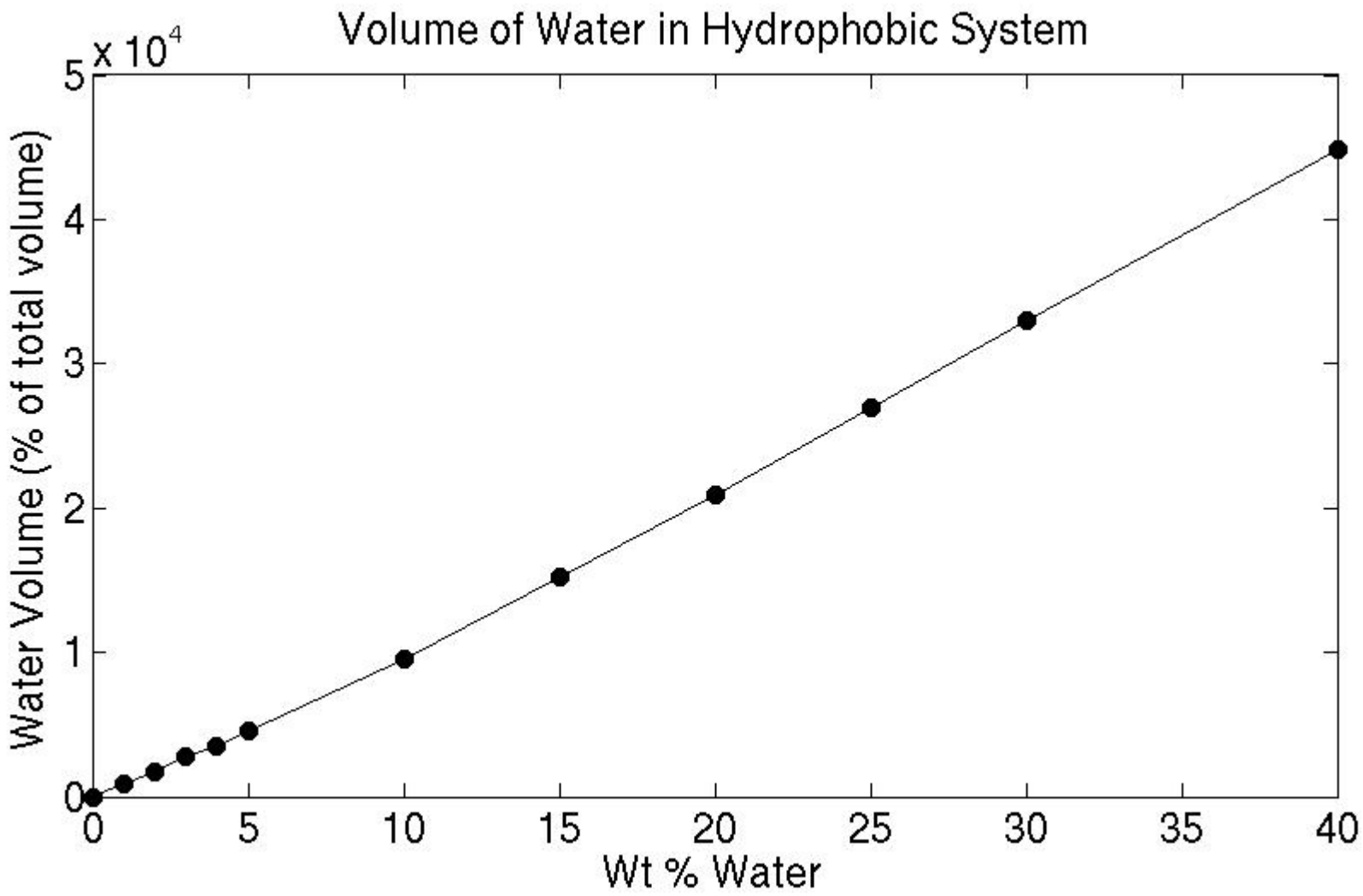
Radius of gyration for each chain in hydrophobic system. Trend consistent with swelling behavior.


Density of Hydrophobic System
1.05
1
0.95
0.9
0.85
Density (g/cm3)
0
10
20
30
40
Wt % Water

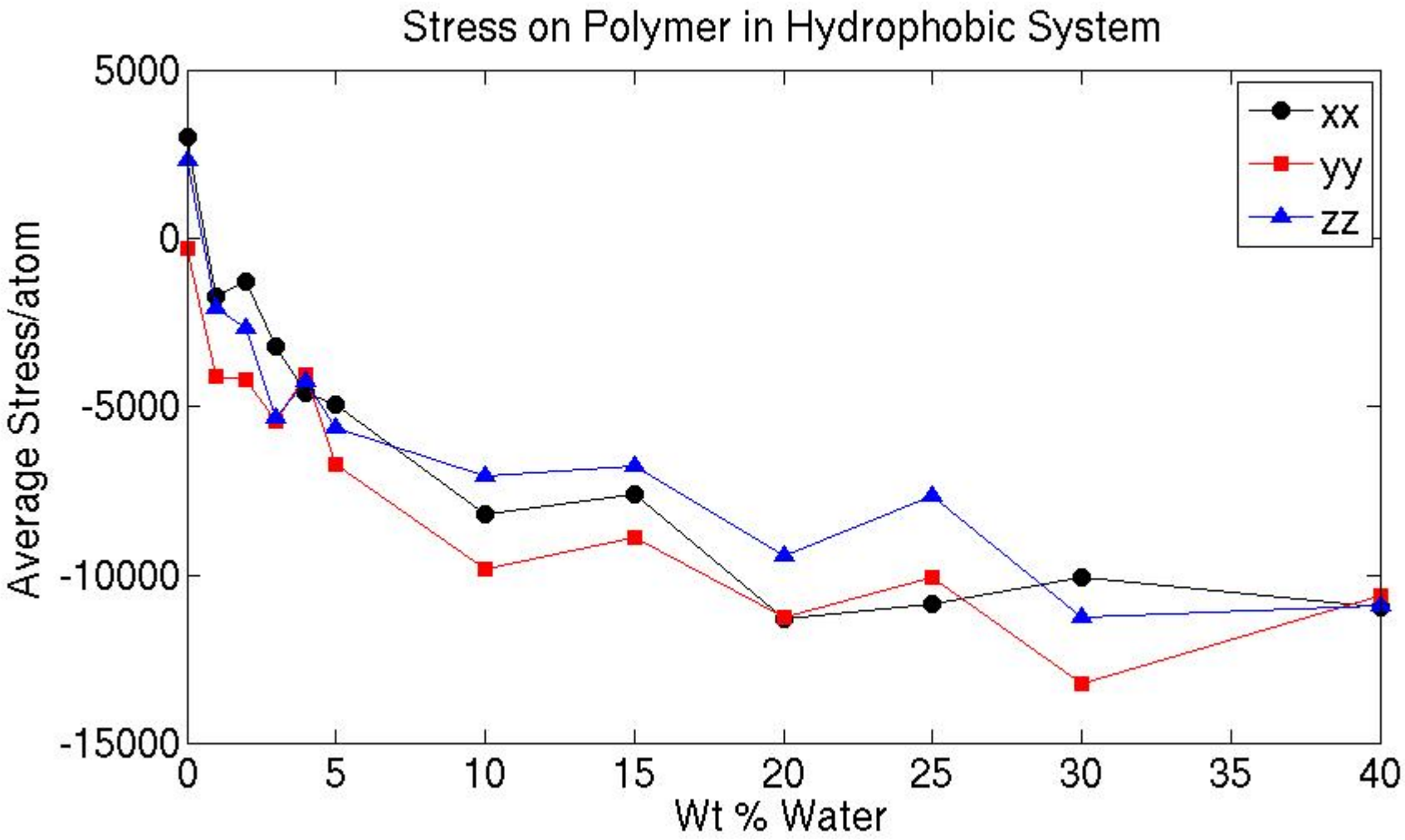

Volume of Hydrophobic System
x 10^5
5
4.5
4
3.5
3
Volume (Angstrom^3)
0
10
20
30
40
Wt % Water



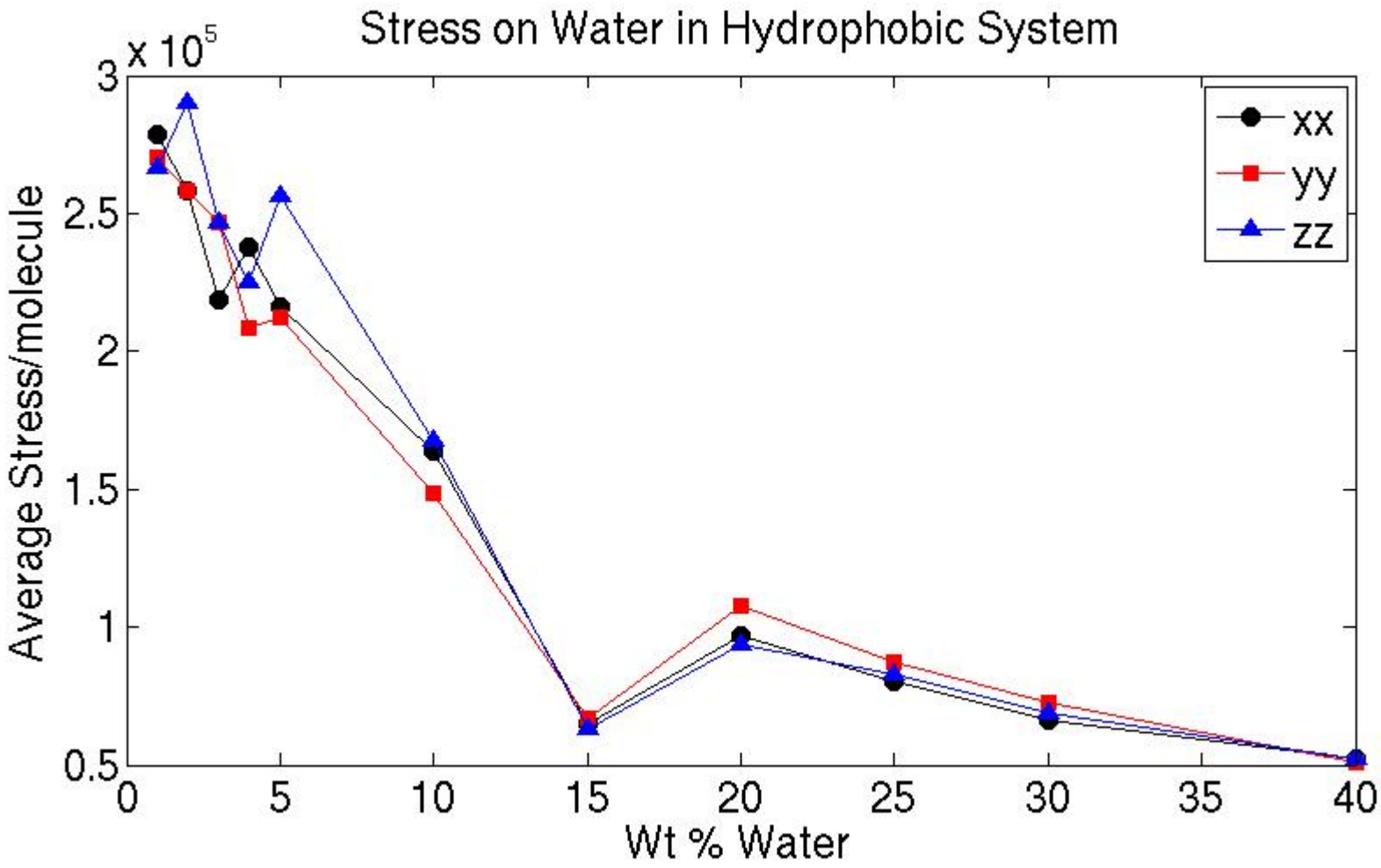
This is true void (ie, empty space) volume. Fraction of empty space decreases as we add more water (the water fills in the voids)



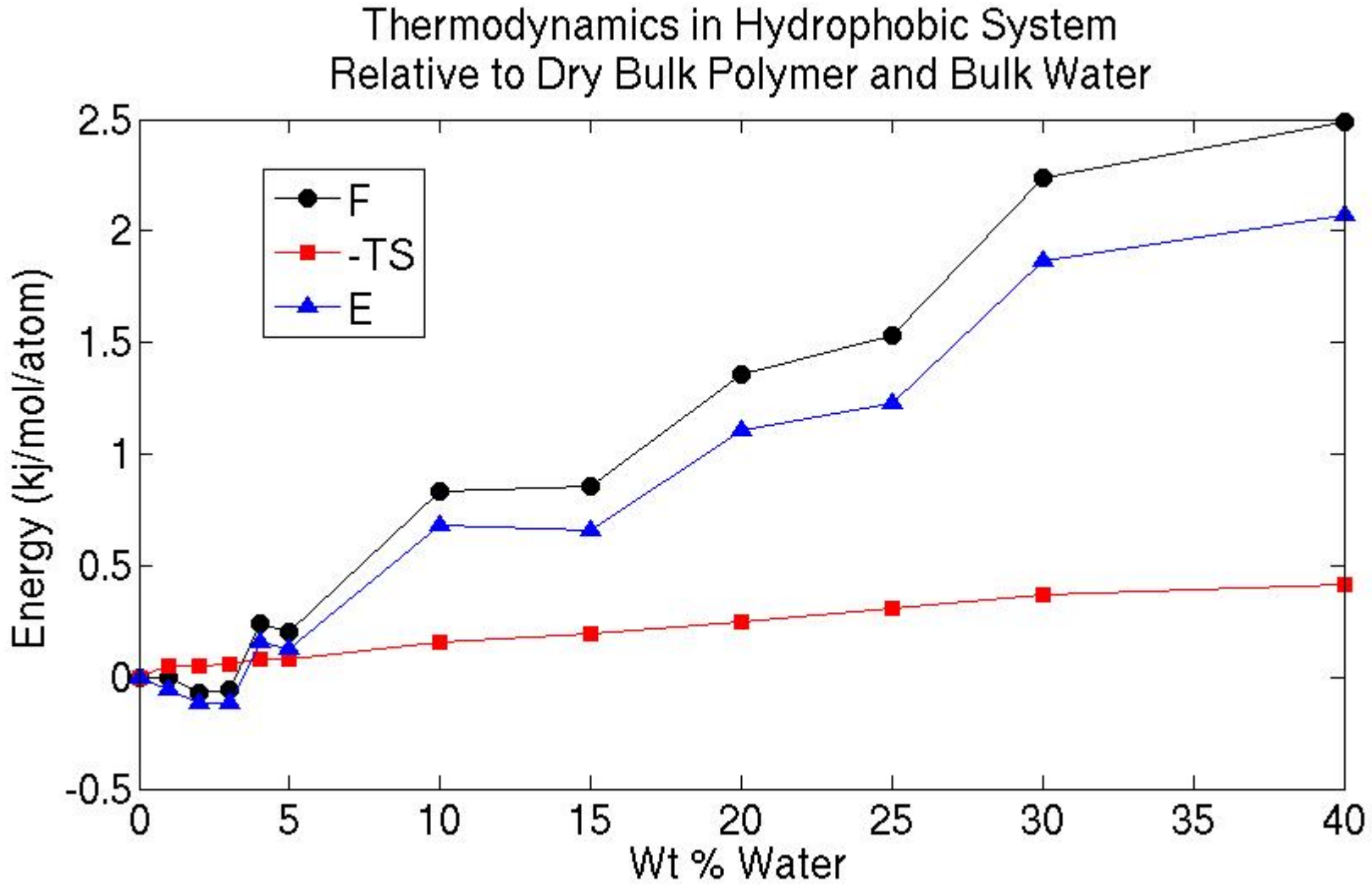
Volume occupied by water increases with water content as expected. Slight kink suggests percolation at ~15-20% (consistent with previous results)



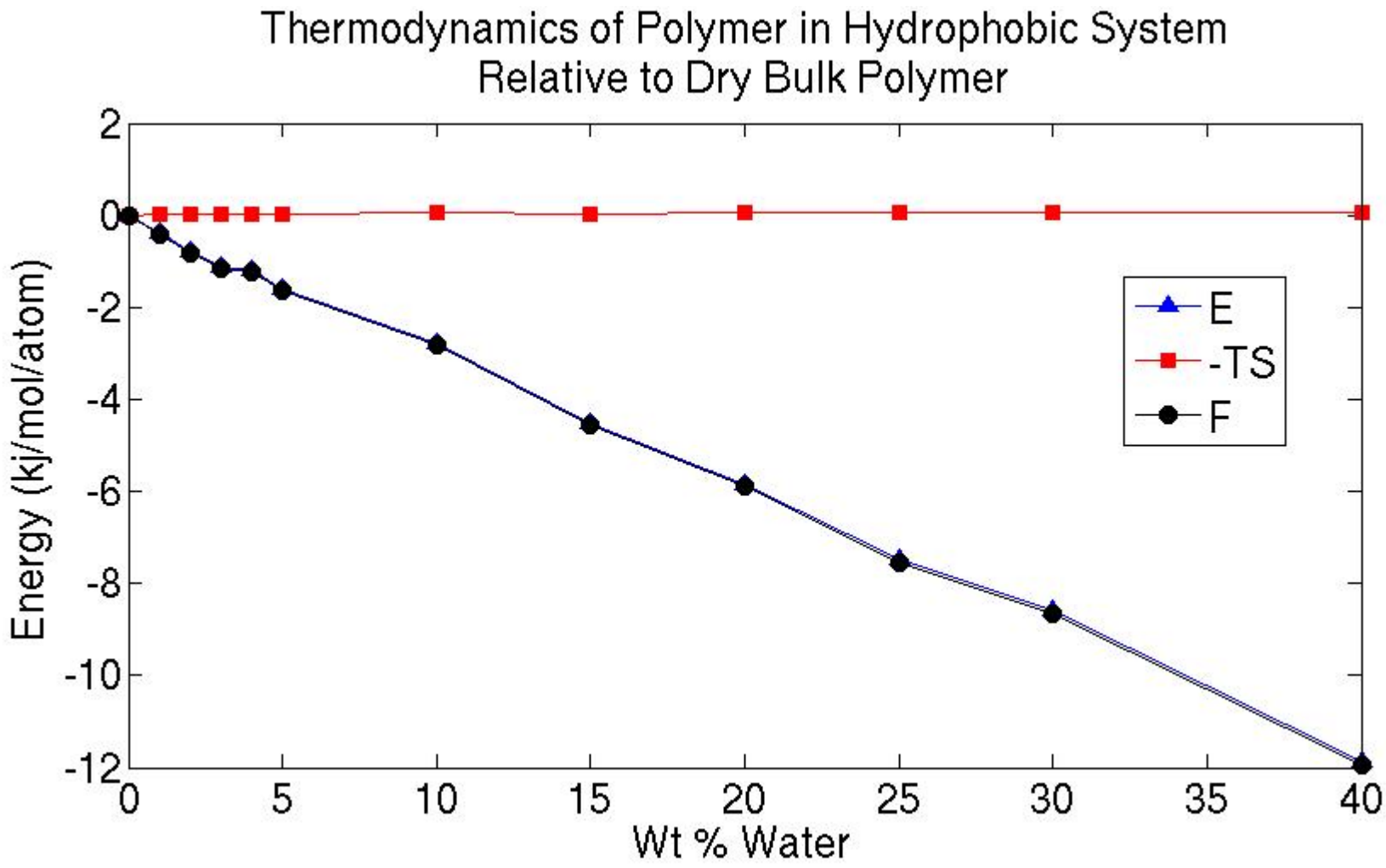
Time-averaged diagonal components of stress tensor of polymer atoms, averaged per atom.
As defined in our calculations, the stress tensor is the negative of the pressure tensor. Note pronounced kink at 20%

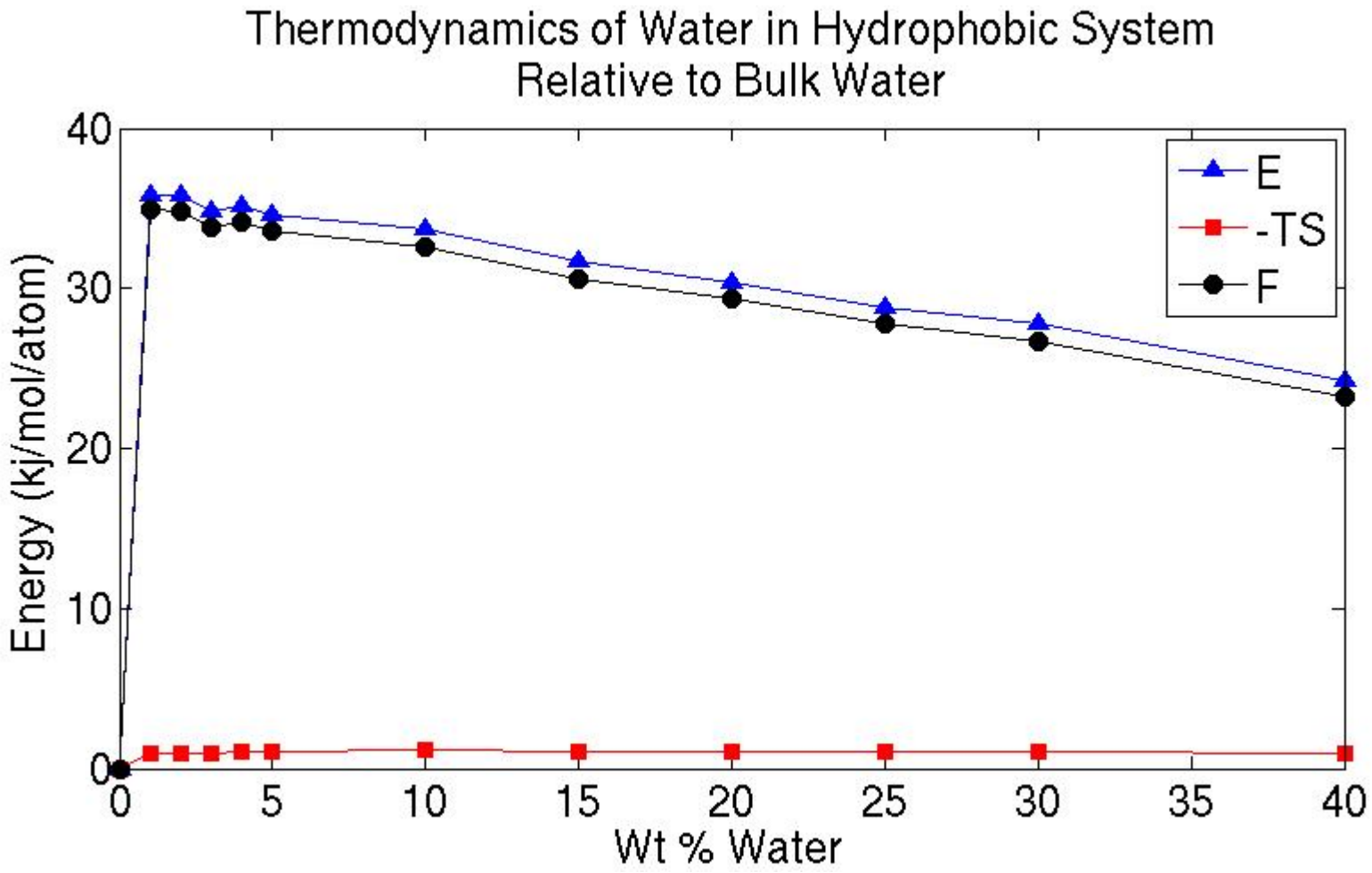


Very similar kink at 15%. Stress on water shows similar trend, opposite sign to stress on polymer.

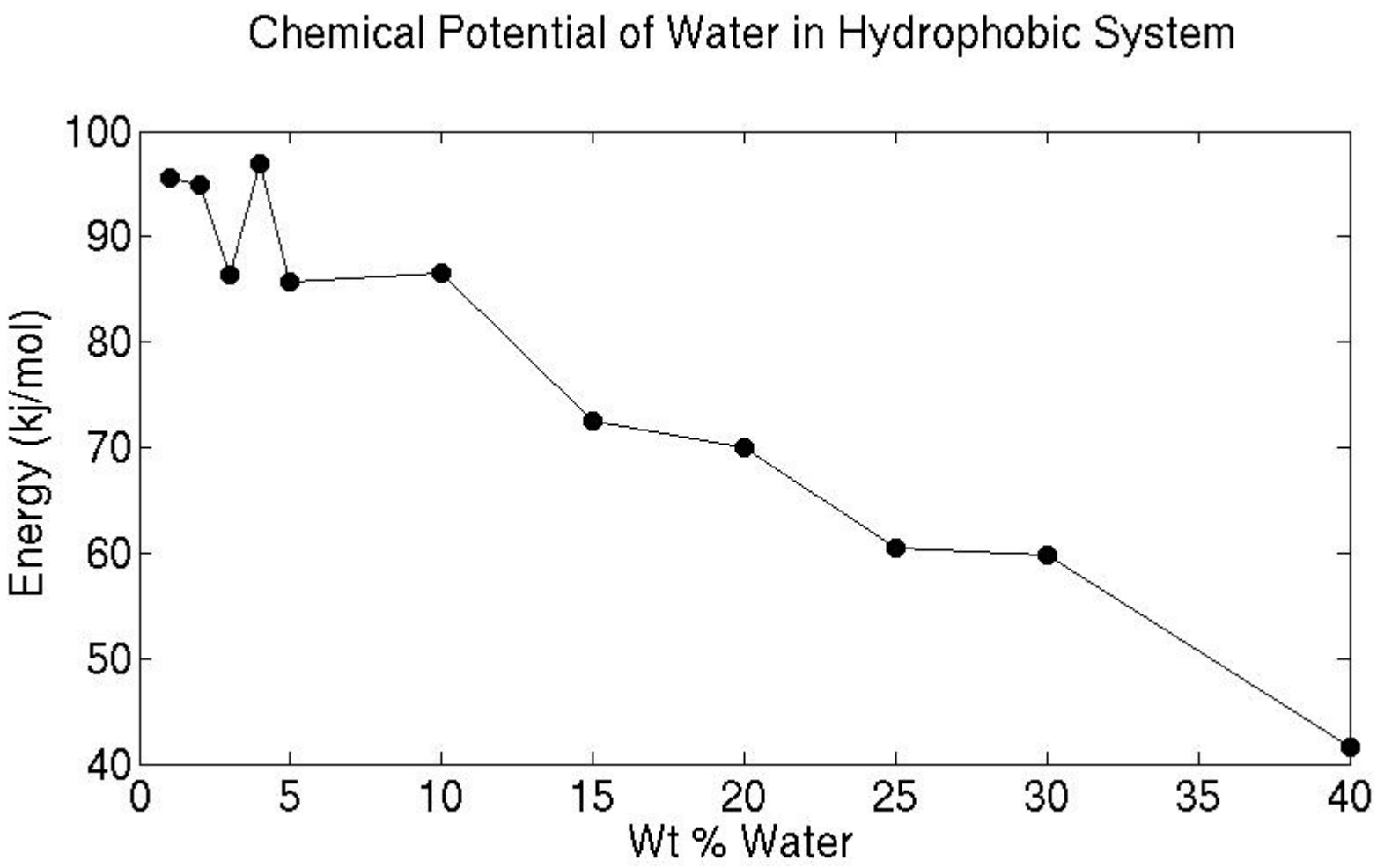


Thermodynamics of entire system. Free energy suggests equilibrium water content ~3-4%. Kink at 20%, perhaps related to percolation. Steady increase in free energy with water content, similar to previous results despite new equilibration procedure.


Thermodynamics of Polymer in Hydrophobic System
Relative to Dry Bulk Polymer
Energy (kj/mol/atom)
Wt % Water
E
-TS
F
2
0
-2
-4
-6
-8
-10
-12
0
5
10
15
20
25
30
35
40



Decrease in free energy with water content is consistent with decrease in stress, formation of hydrogen bonding network, decrease in interface between polymer and water.


Chemical Potential of Water in Hydrophobic System
Energy (kj/mol)
100
90
80
70
60
50
40
0
5
10
15
20
25
30
35
40
Wt % Water