Latex Films

Dow Chemical Project

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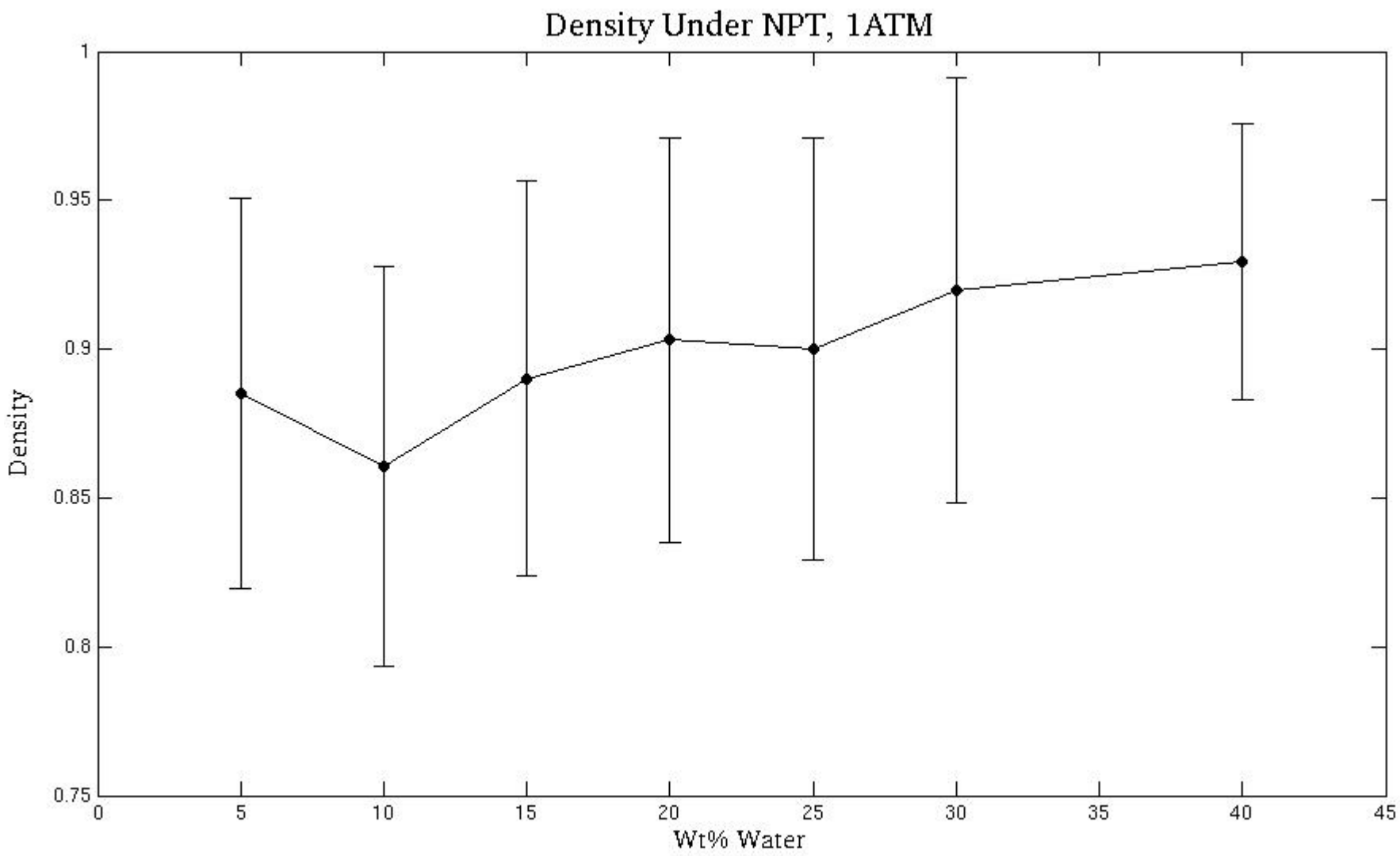
DOW Chemical 7-13-3011

Thermodynamics of Solvated Hydrophobic System

- Added water molecules at random positions to 40 wt. %
- CED
- Randomly remove water molecules to make 30,25,20,15,10,5,0 wt % structures
- Thermodynamics (entropy, free energy by 2PT) for all at three densities

Motivation

- Characterize free-energy, entropy and enthalpy as a function of water content



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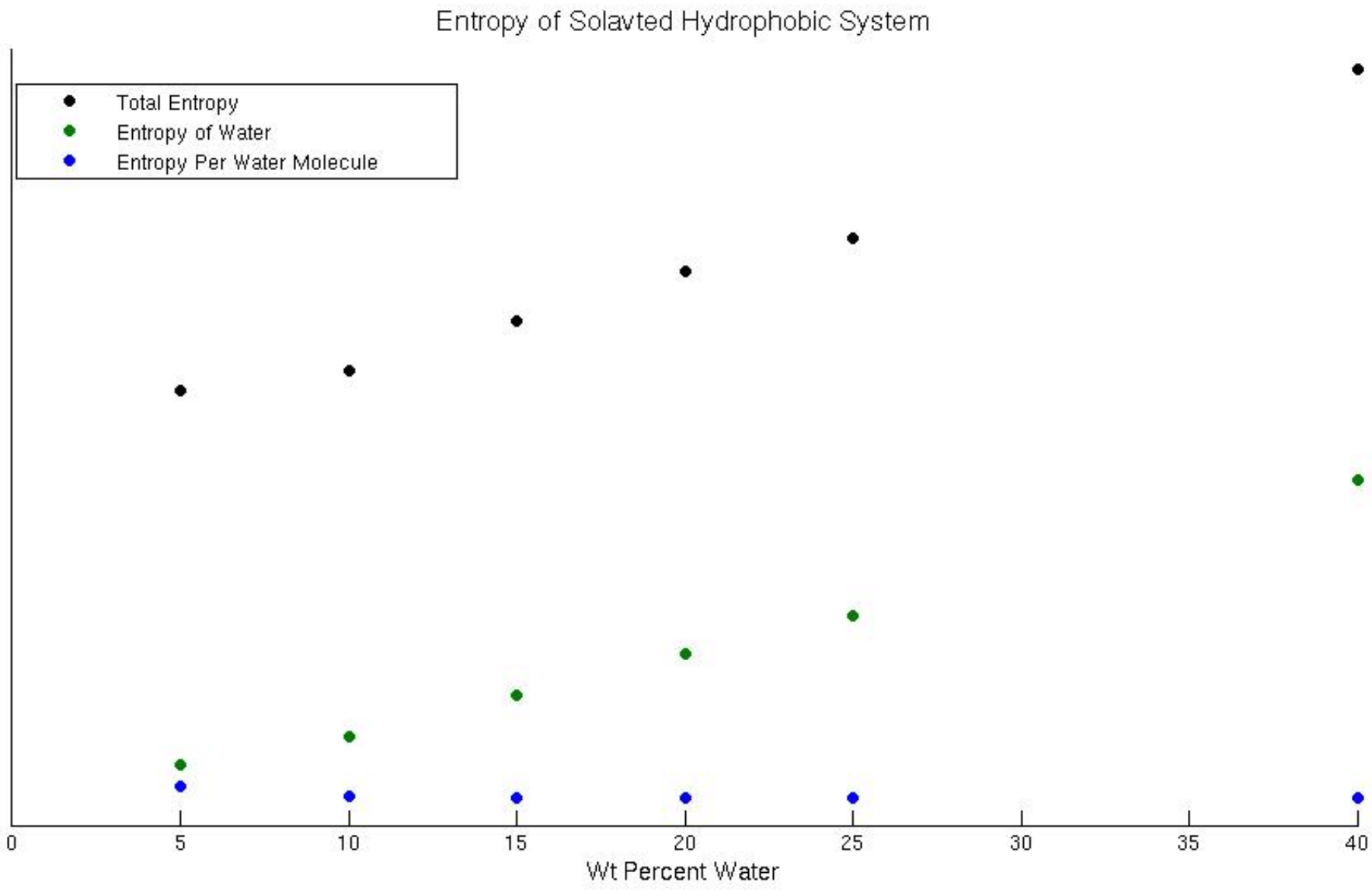

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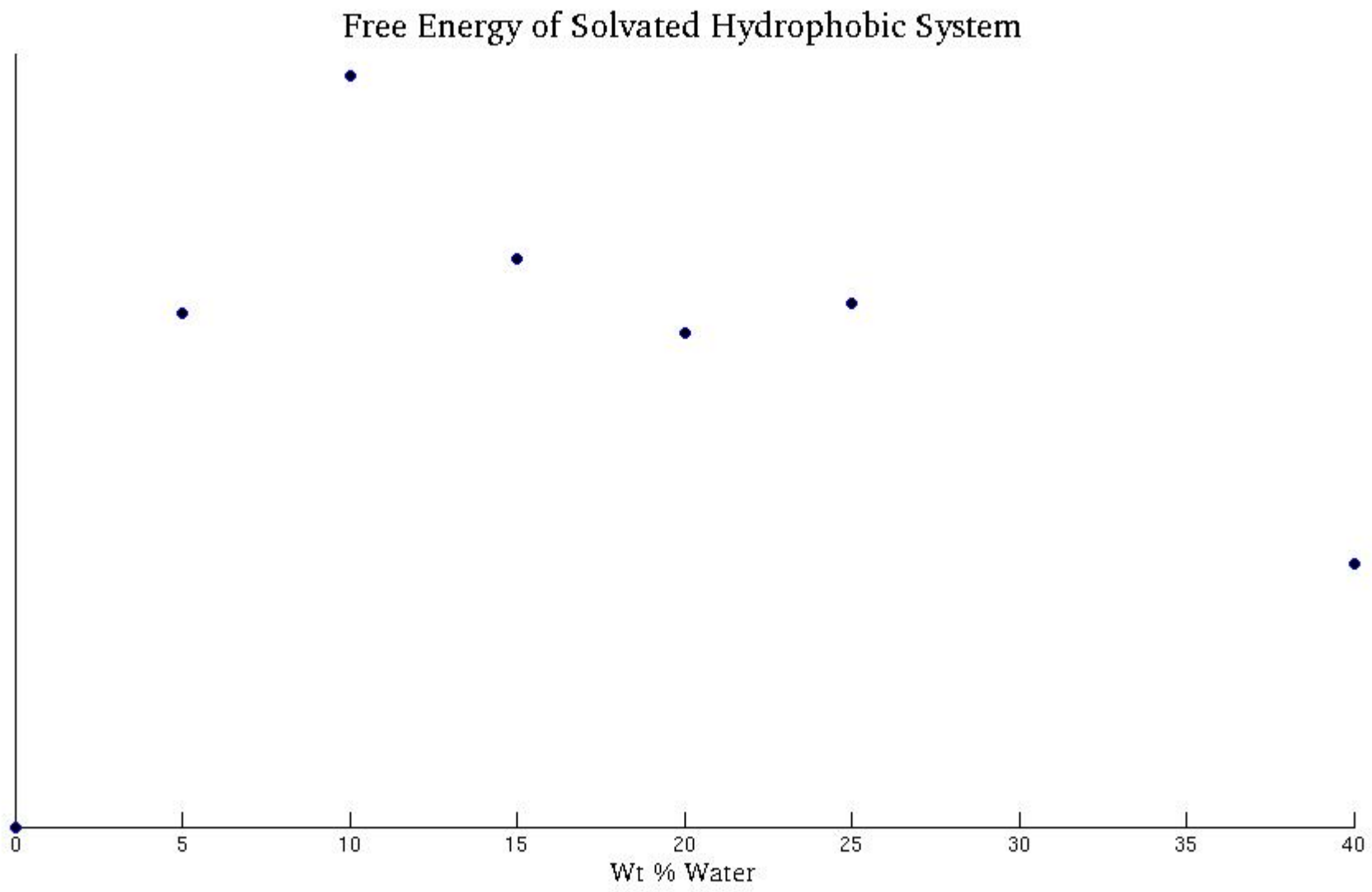

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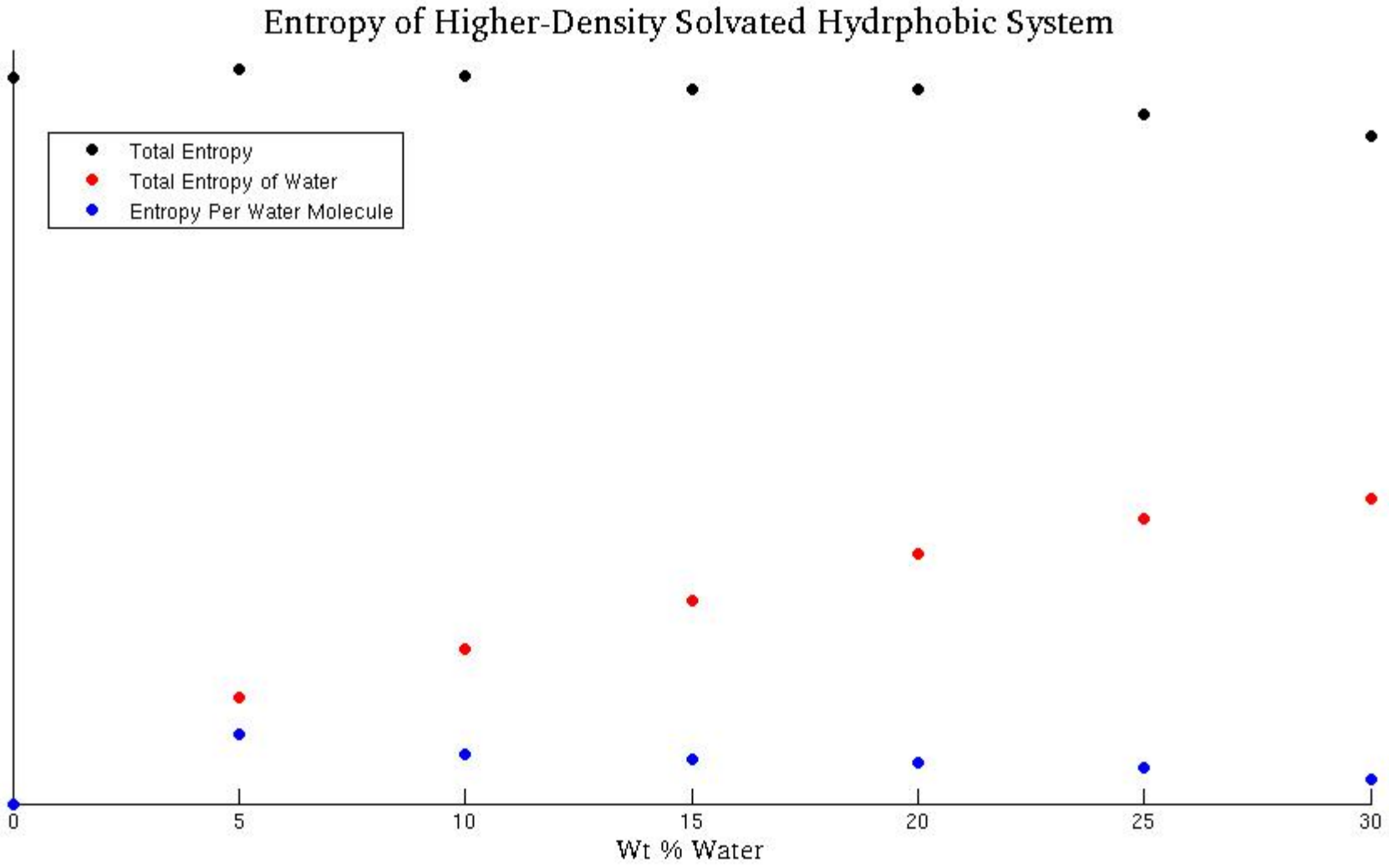

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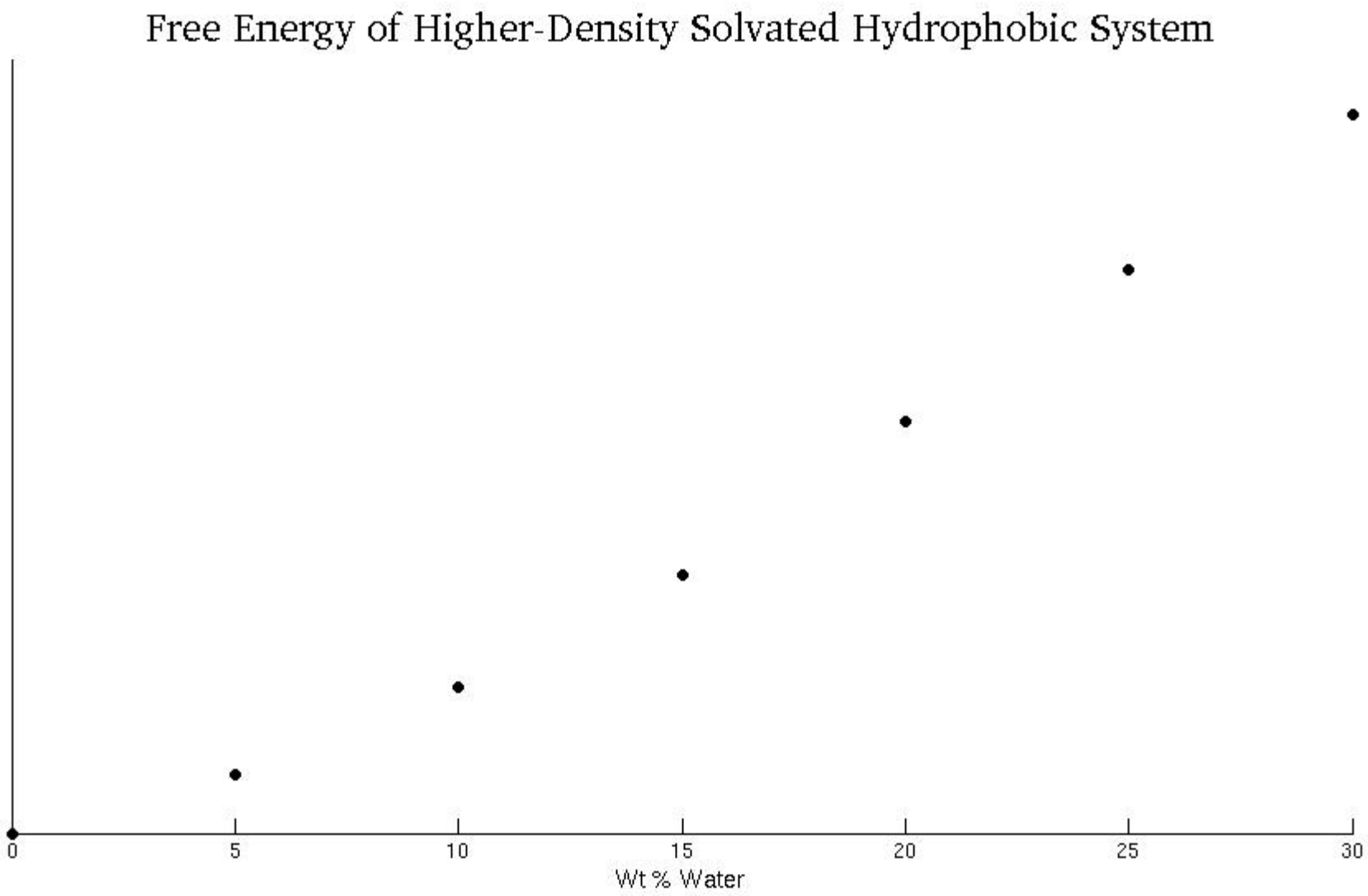

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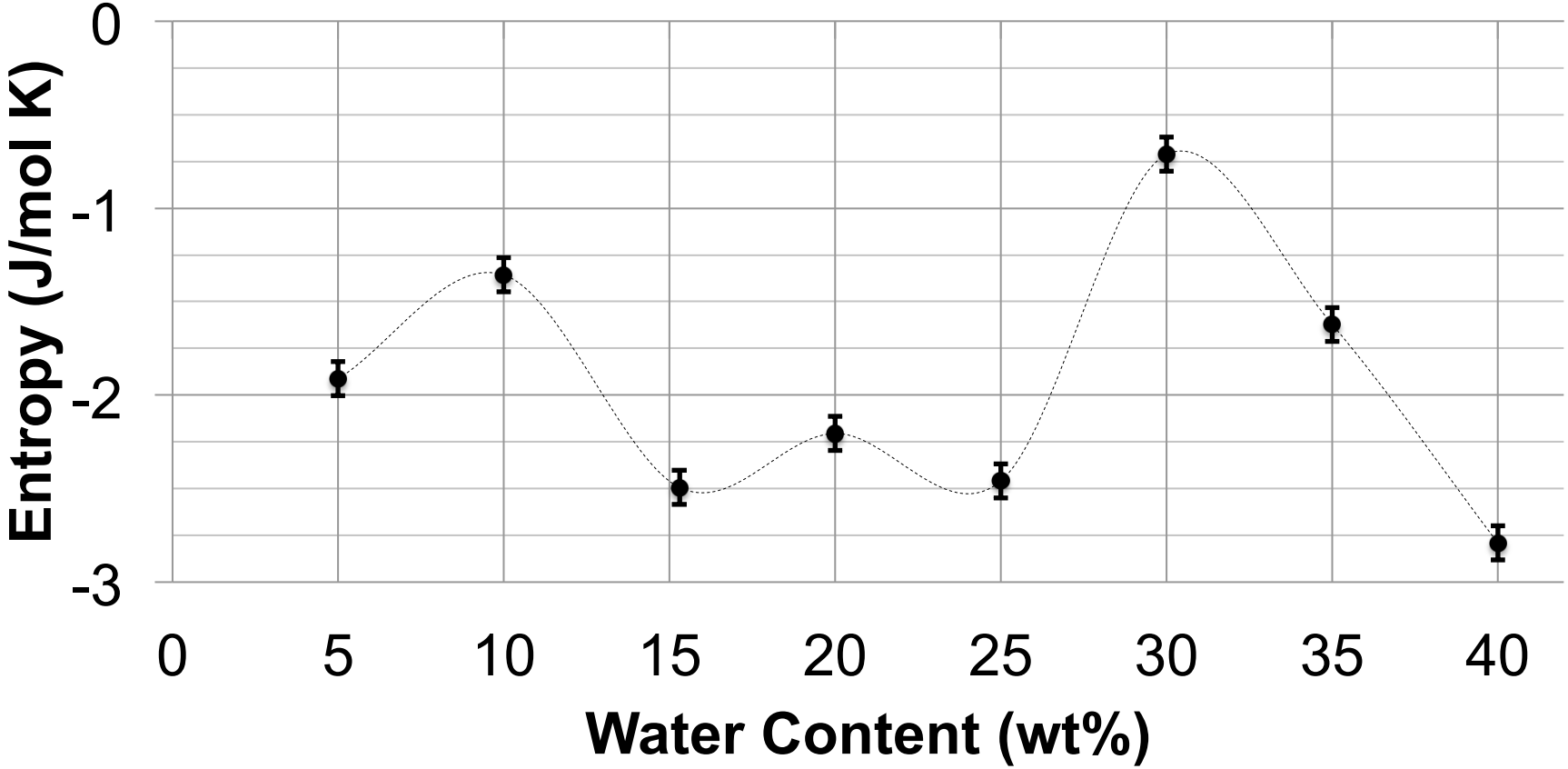
Thermodynamics of hydrophilic system

- For the data plotted here:
- Hydrophilic System Composition
- DREIDING Polymer, F3C Water
- Lennard-Jones, fixed partial charge, hydrogen-bonding between MMA* and water

- 2PT data gathered for 20ps at 4fs intervals, NVT @ 300K and 1 g/cc
- 9163 polymer atoms

- **Entropy Reference** – Bulk Water (F3C => 62.18 J/mol K), Vacuum Polymer
- **Internal Energy Reference** – Bulk Water (F3C => -9.6 kcal/mol [-40.1664kJ/mol]), Vacuum Polymer
- **Free Energy** = H-T*S DOW Chemical 7-13-3011

Water Entropy, Per Atom - Hydrophilic System (1g/cc)



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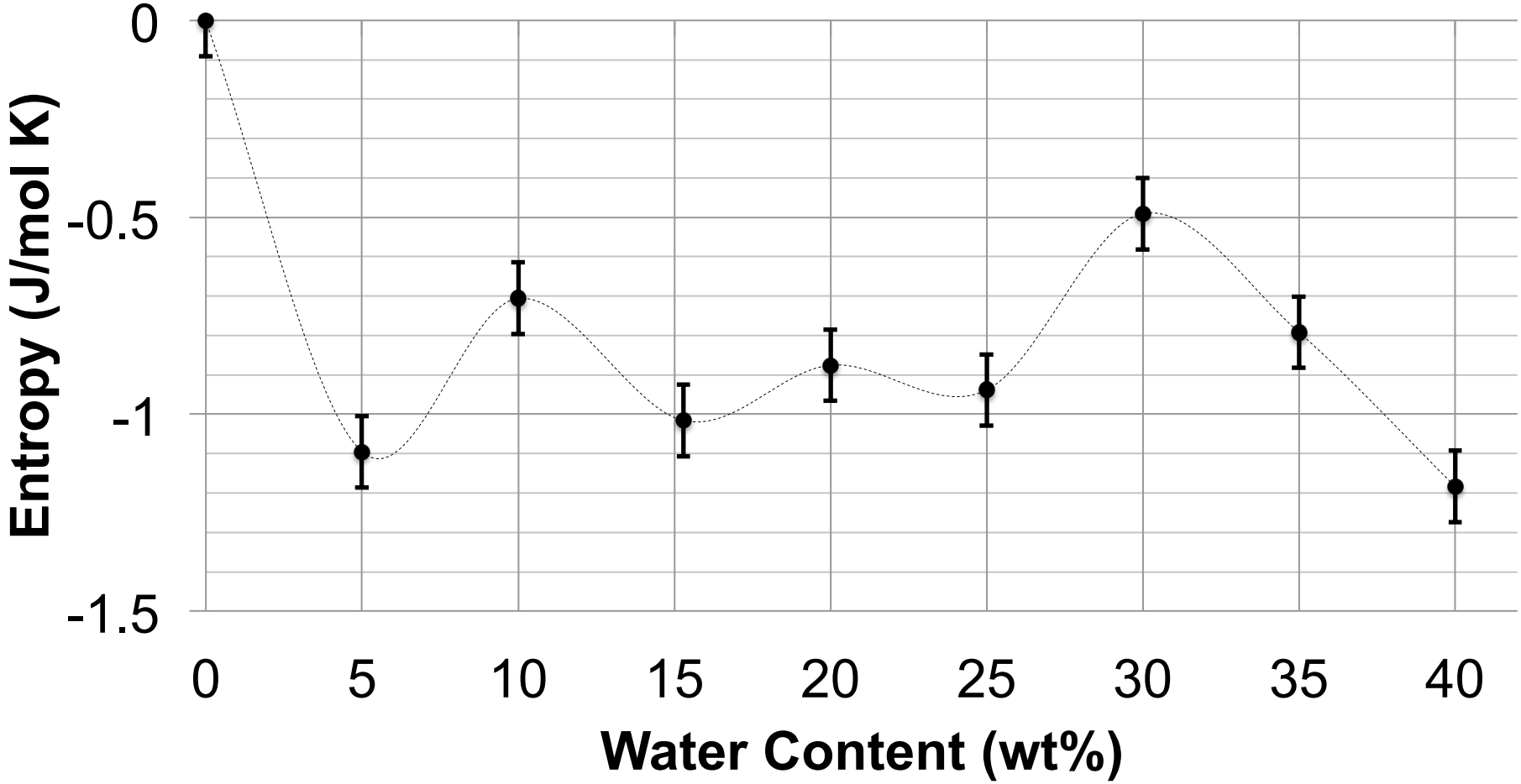
Polymer Entropy, Per Atom - Hydrophilic System (1g/cc)



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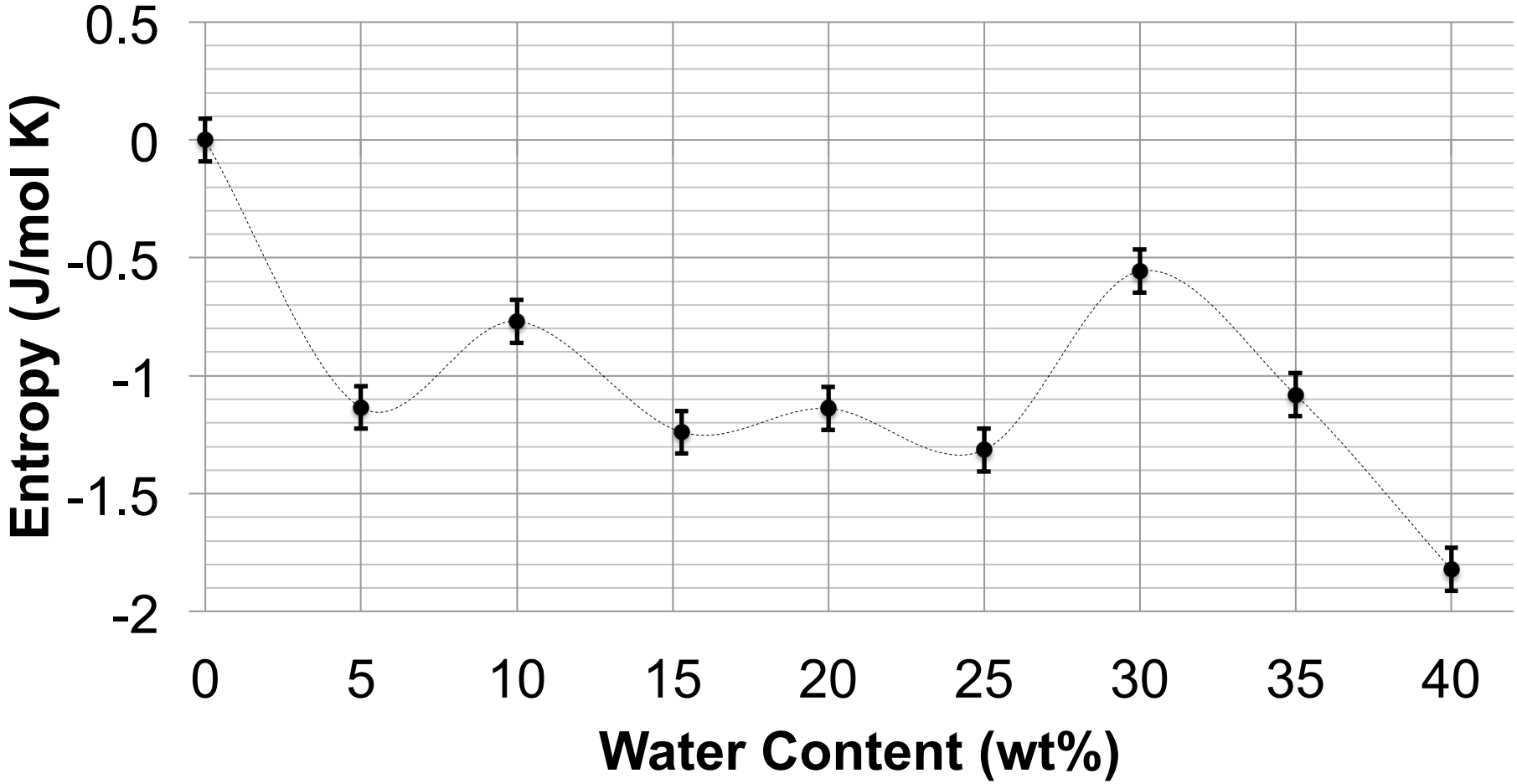
Total Entropy, Per Atom - Hydrophilic System (1g/cc)



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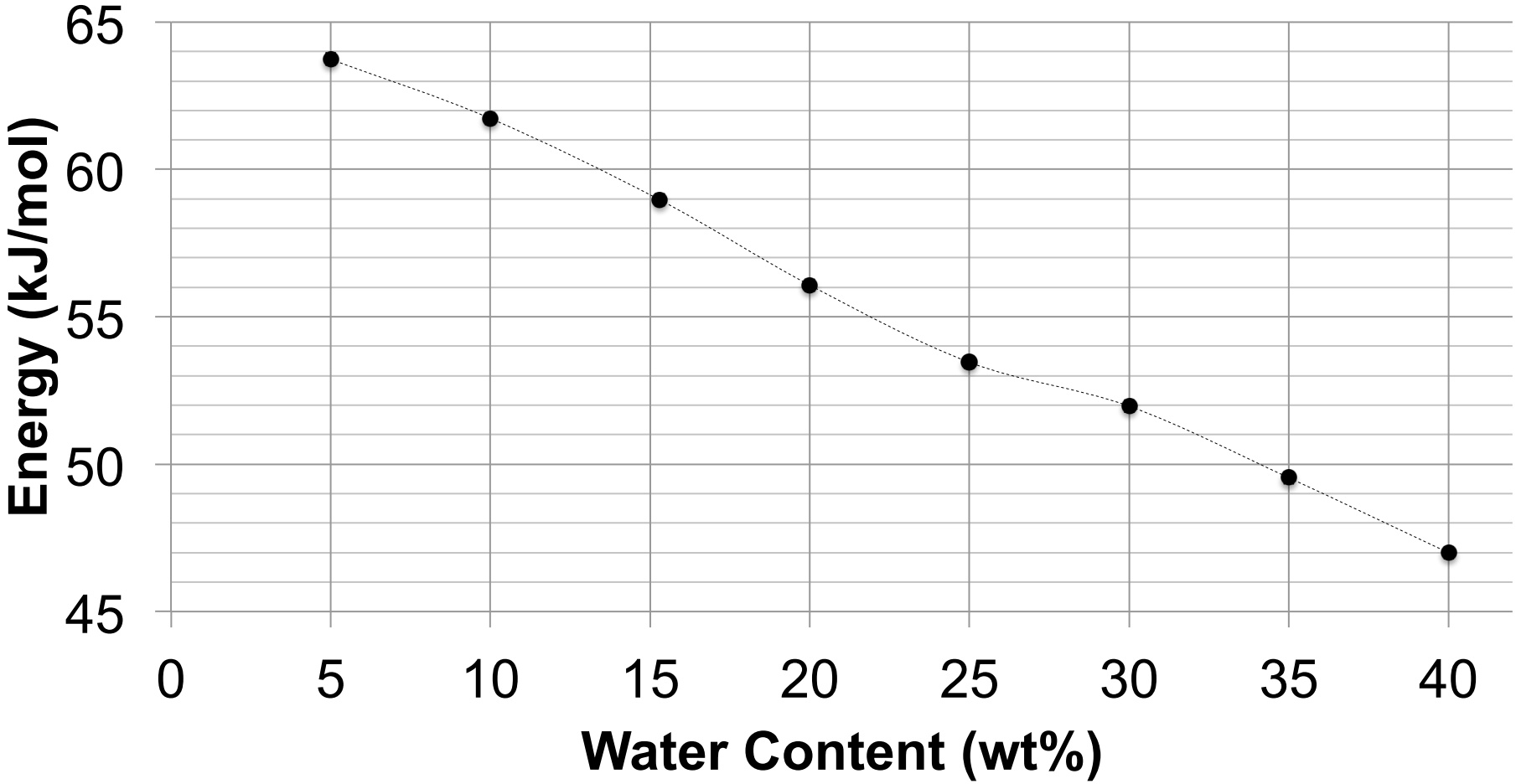
Water Enthalpy, Per Atom - Hydrophilic System (1g/cc)



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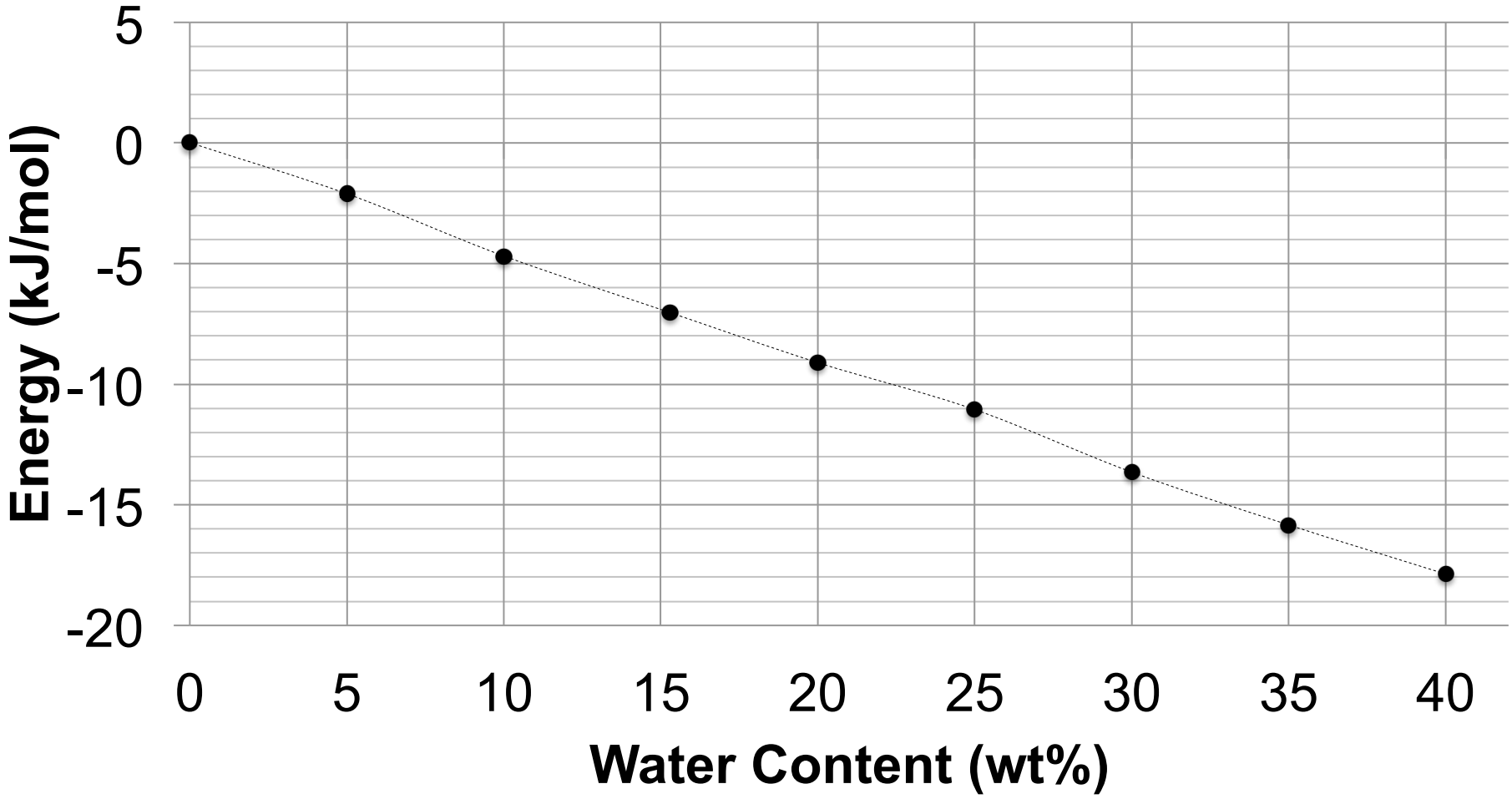
Polymer Enthalpy, Per Atom - Hydrophilic System (1g/cc)



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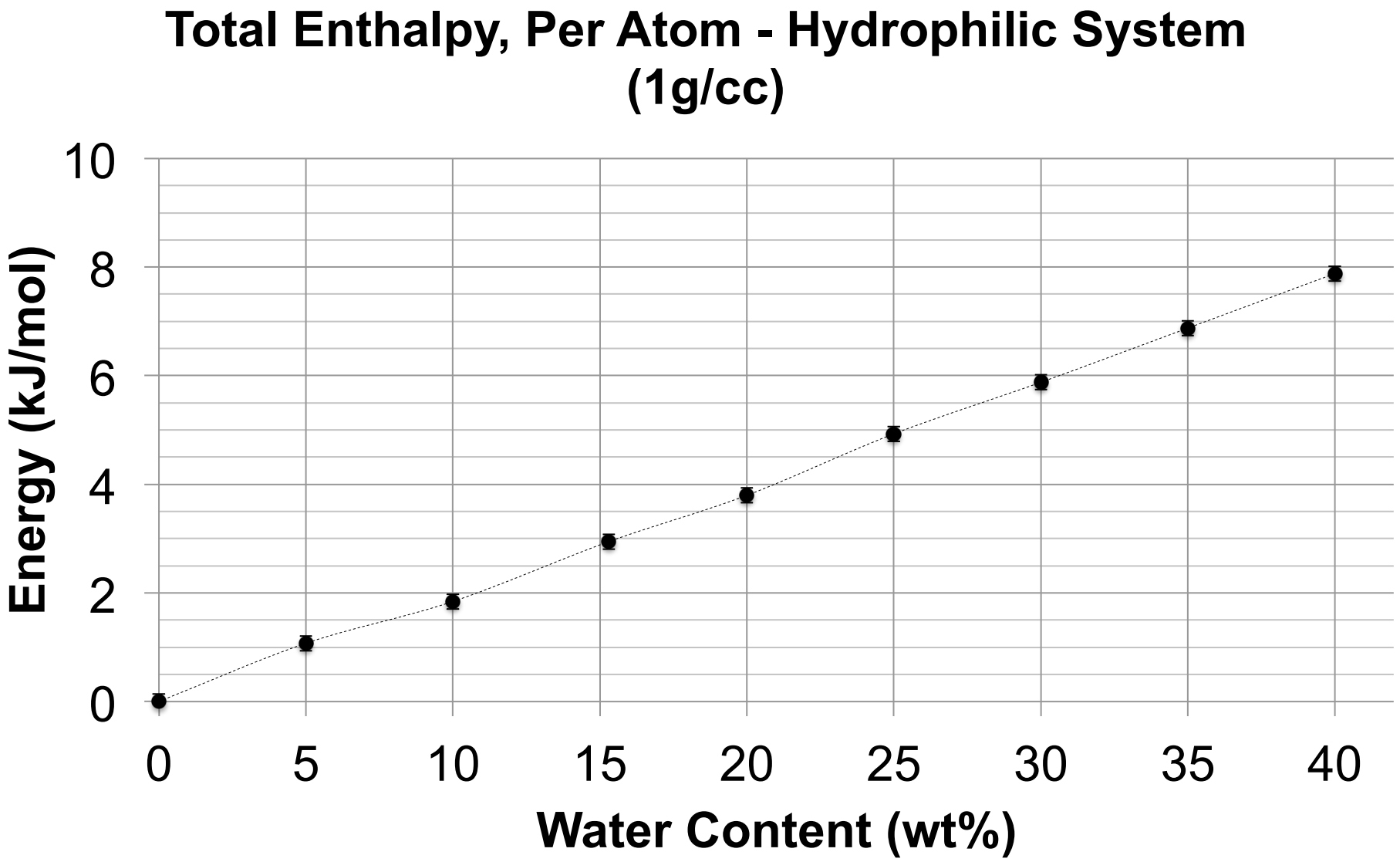

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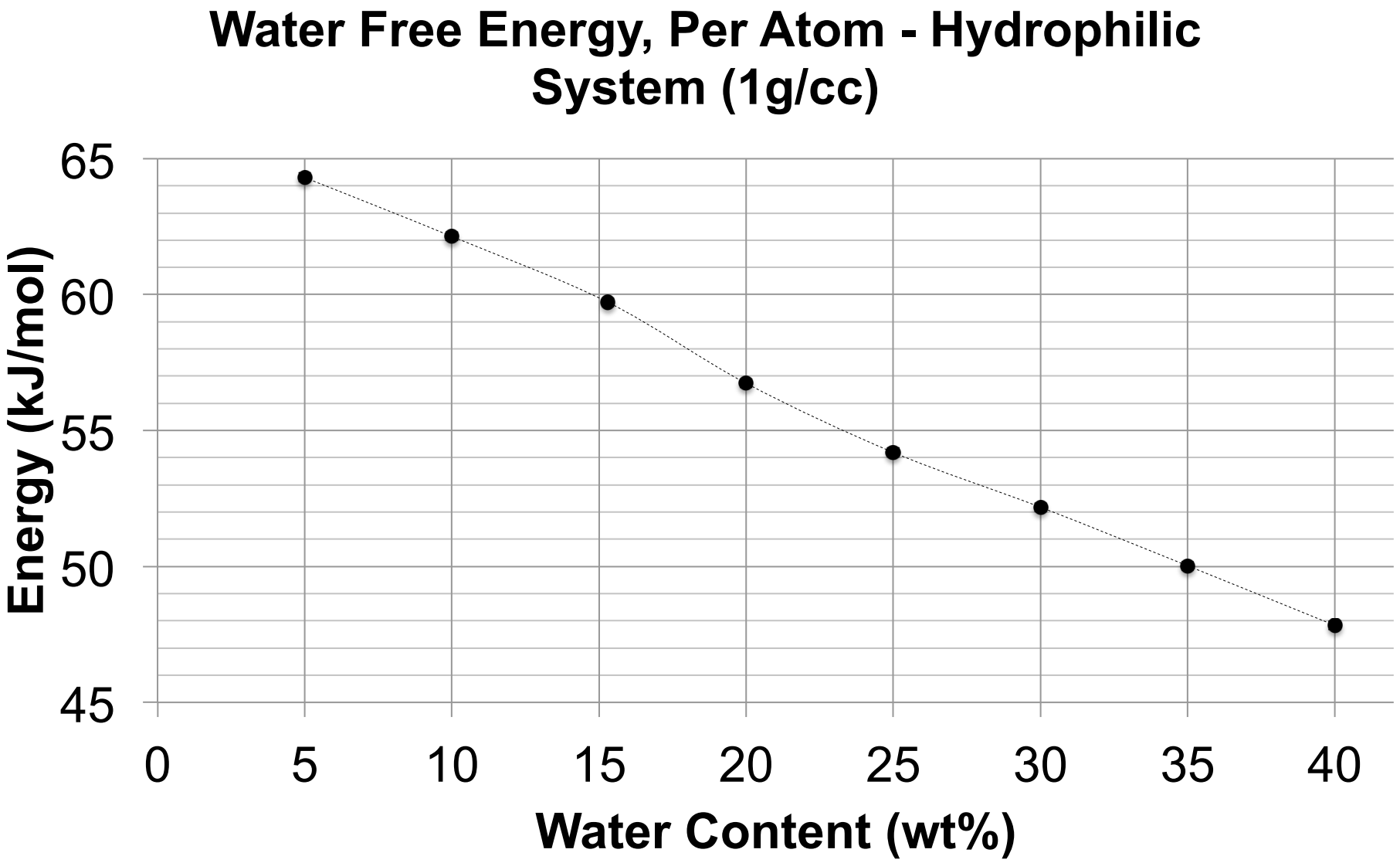

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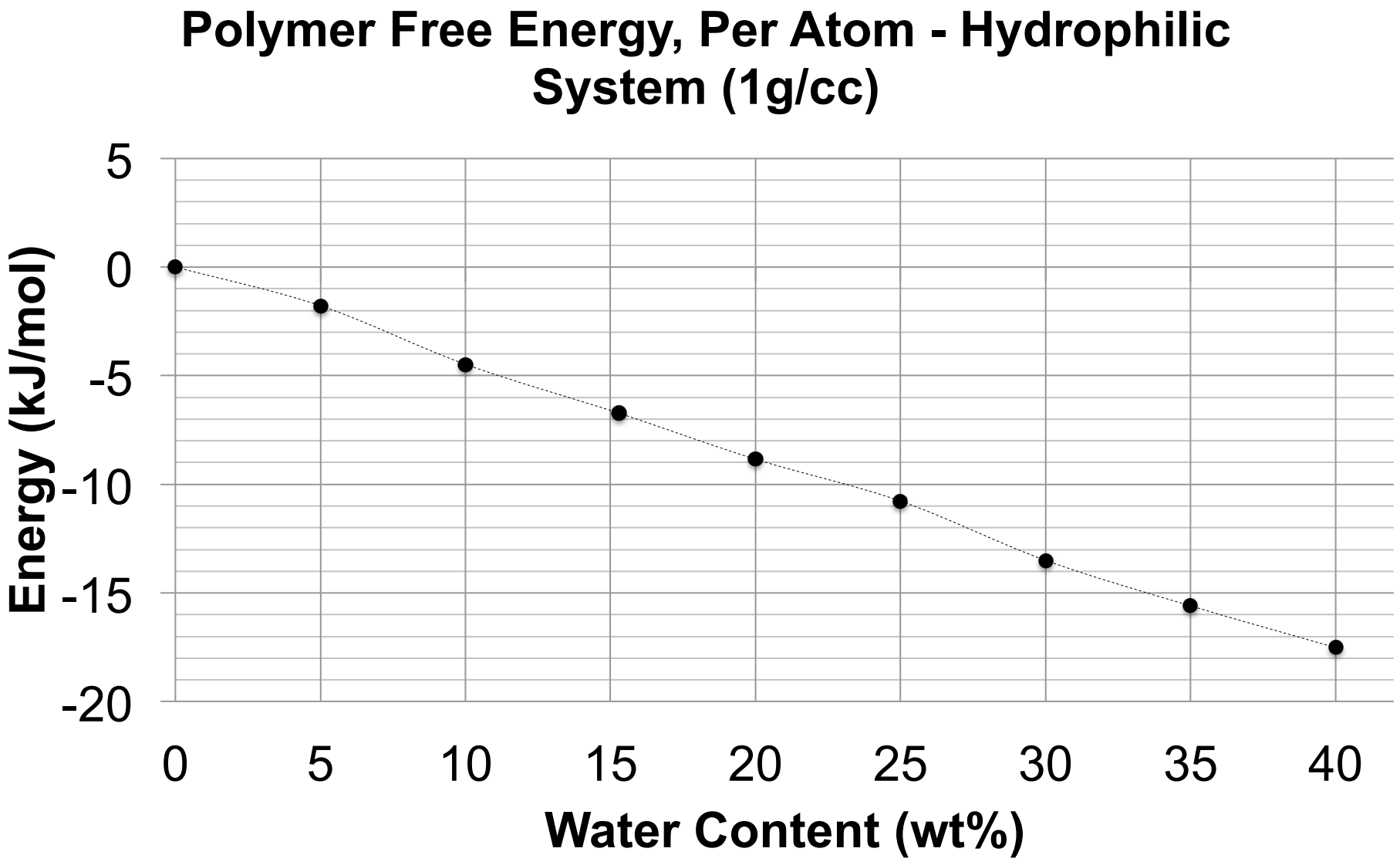

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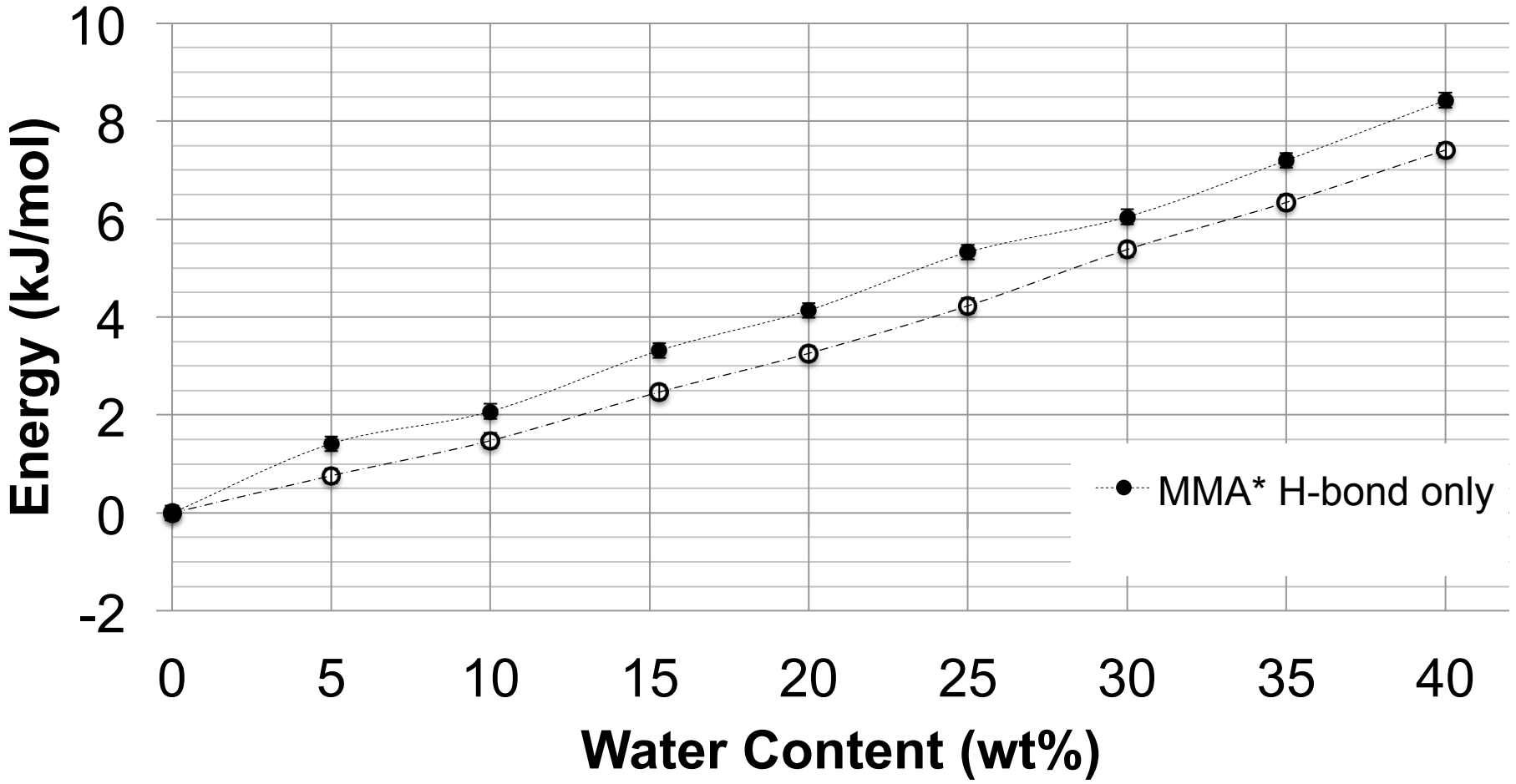
Total Free Energy, Per Atom - Hydrophilic System (1g/cc)



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