

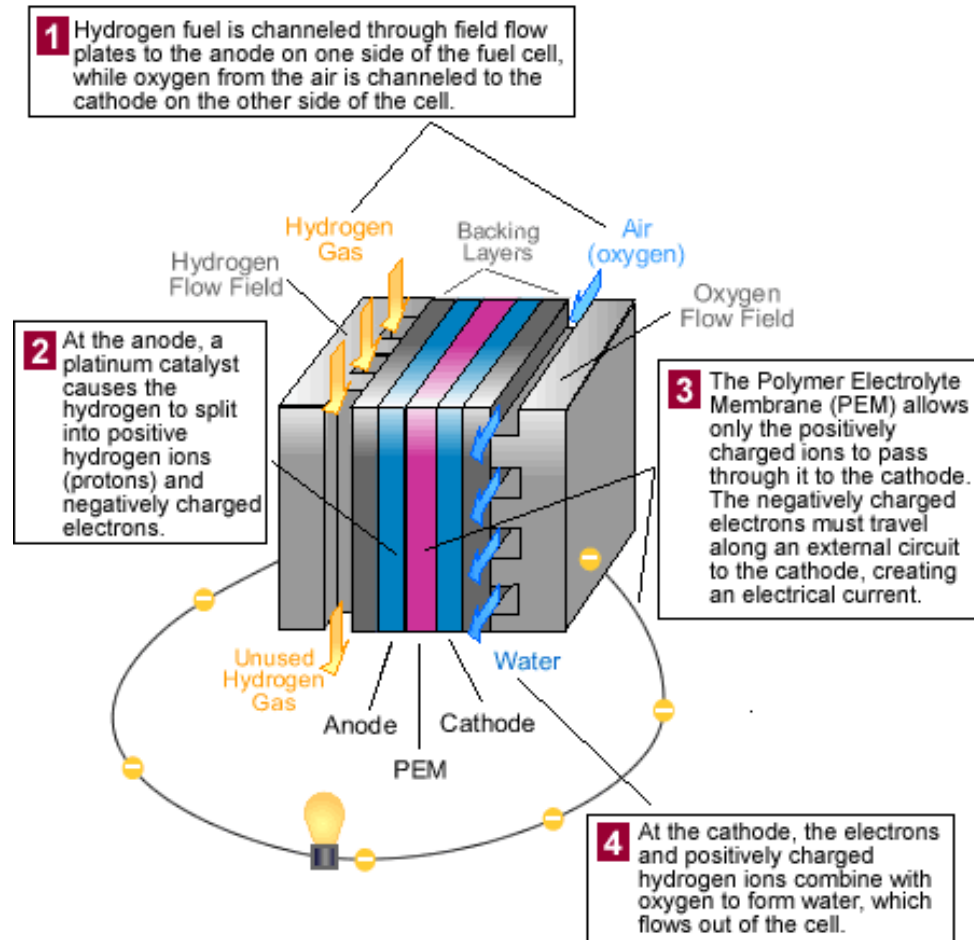
Hydrogen Storage: Simulations on LaNi_5H_6

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Why is it important?

- Fuel Cells!



Monte Carlo Simulations

- Propose a change to an existing system (e.g. position of a particle or addition/removal of a particle)
- Calculate probability (of being at the current position, of the possibility of moving to the new position, and of actually moving to the new position)
- Based on this probability, accept/reject the change

Our Simulation

- We use a Grand Canonical (μ, V, T) Monte Carlo Simulation
- Monitor change in:
 - Number of particles
 - Energy of the system
 - ΔE of adsorption/desorption of H

Objective

- Obtain a reasonable force field
- Optimizing storage conditions:
 - Temperature (the closer to room temperature the easier to achieve)
 - Pressure (the closer to atmospheric pressure the safer)
 - Weight (the lighter the easier to transport)
 - ΔE of adsorption/desorption (ease of storage/release of Hydrogen)

Results

