# Mapping the carbon nanotube formation parameter space: Data mining and mechanistic understanding for efficient resource use

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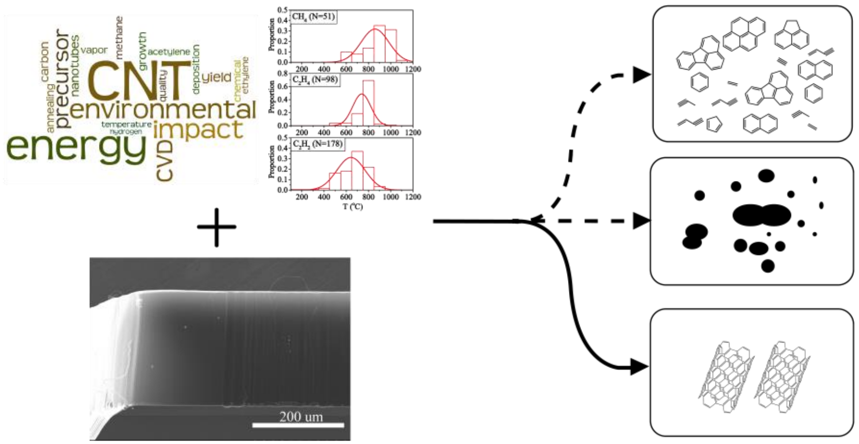


# CNTs in Spotlight

## Booming interests

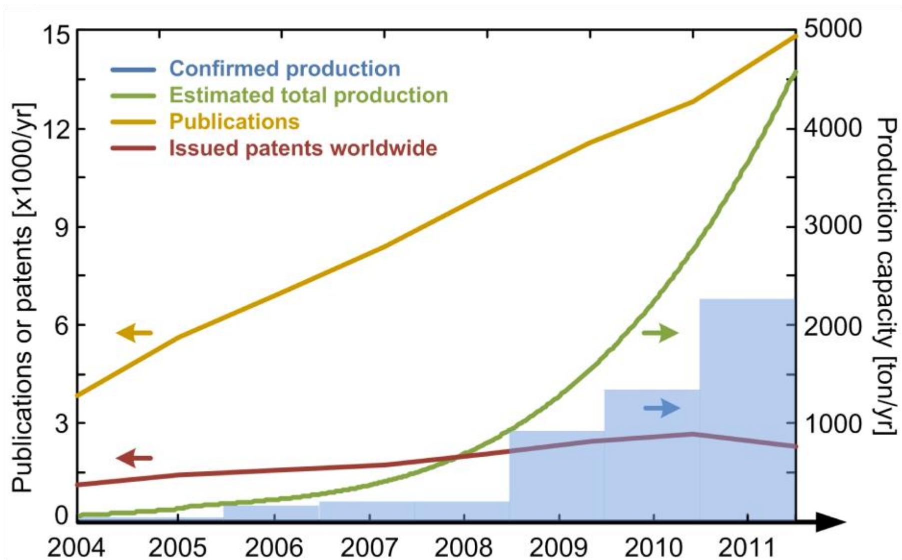


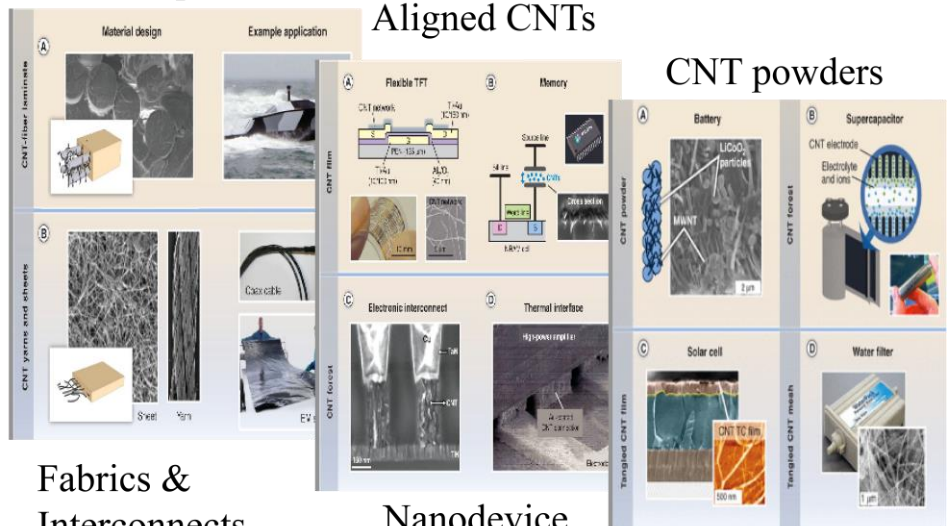

Image Courtesy of De Volder Group at Cambridge

## Widespread applications

Composite

Aligned CNTs

CNT powders




Fabrics & Interconnects

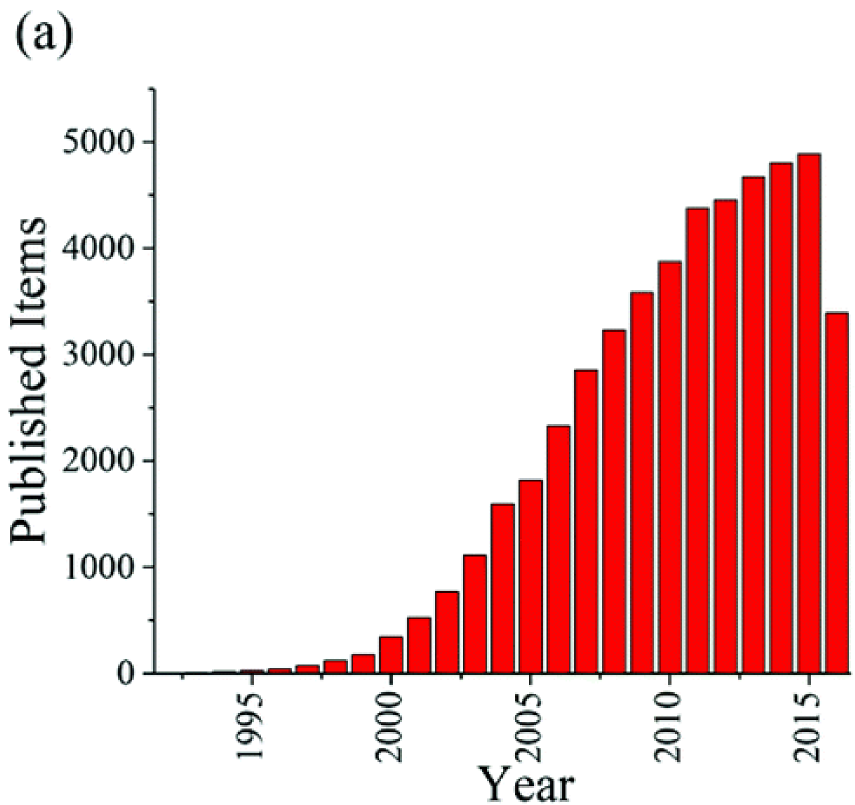
Nanodevice

Environmental & Energy

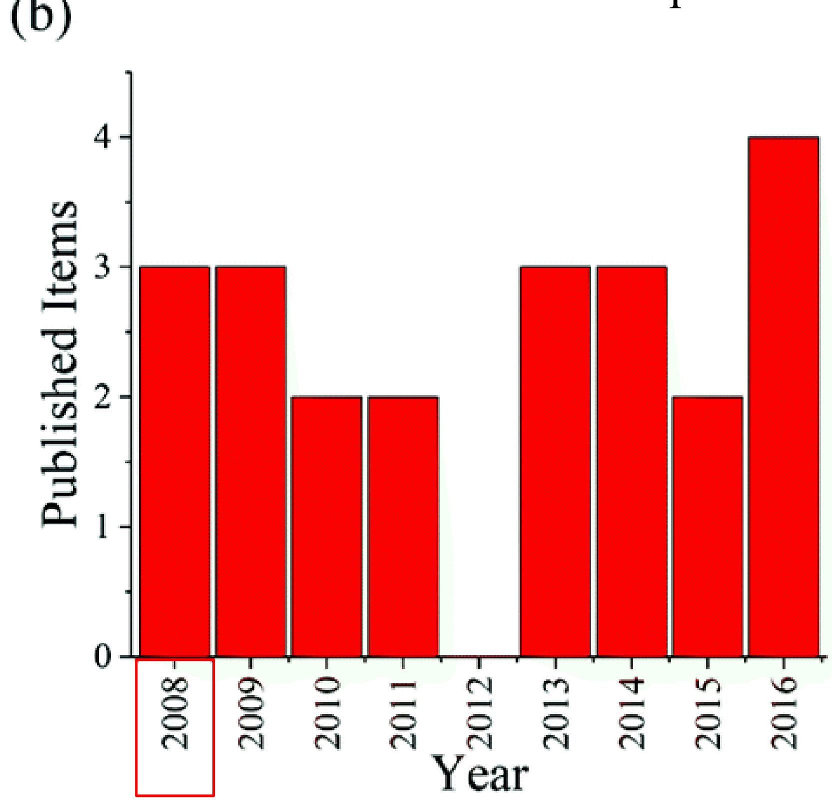
De Volder et al. Science, 2013

# Delayed Environmental Investigation

Topic: “carbon nanotube”




Topic: “carbon nanotube”
AND “environmental impact”

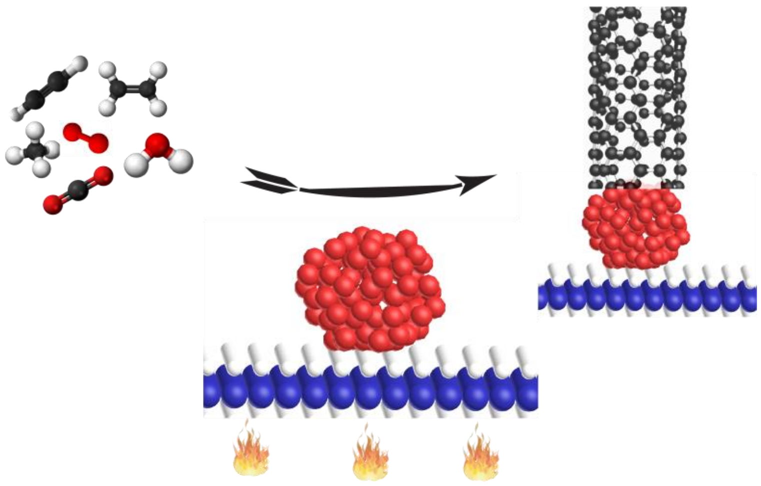



ISI Web of Science database
partial data for 2016

Shi *et al*. Green Chemistry, 2017

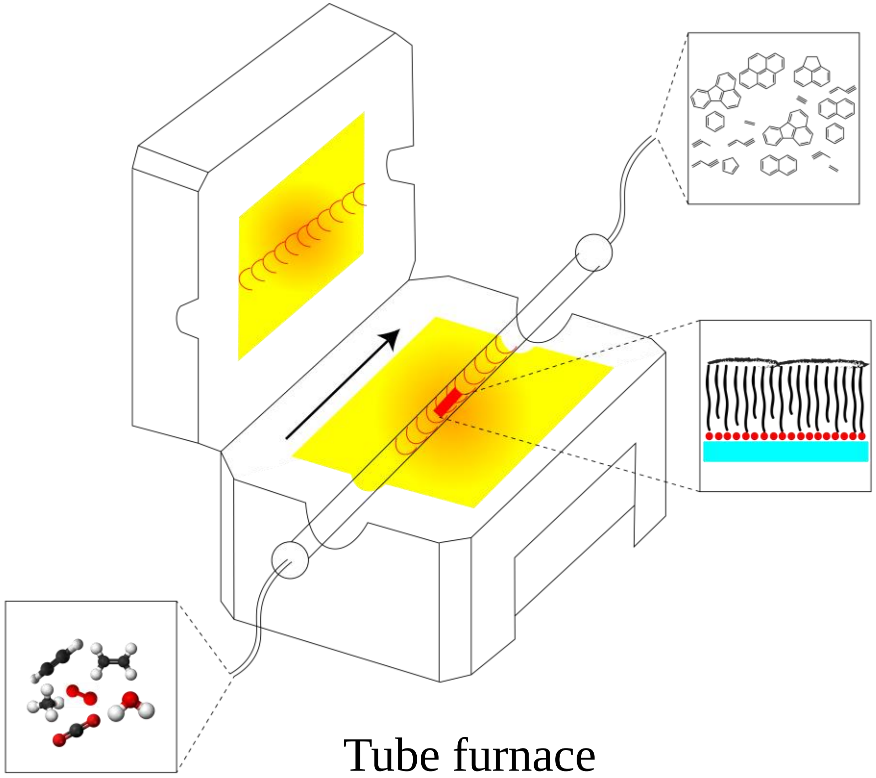
# Sustainable CNT Production Challenges: Energy and Resources

Chemical Process



Heterogeneous catalytic interface

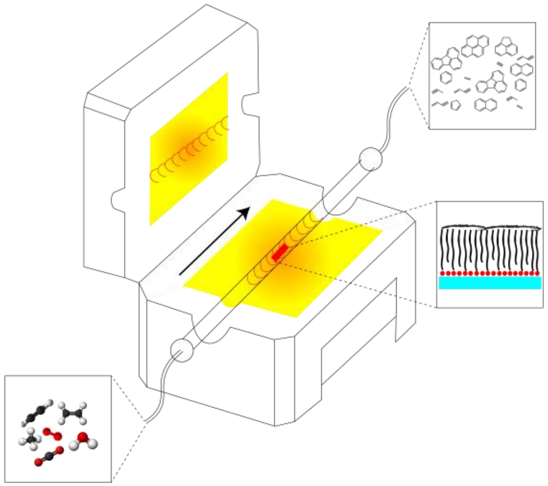
Operating system



Tube furnace

# Address Challenges: Looking Backward

Backward:
- universal mechanistic insights might exist inside widespread recipe formulations
- inform green synthesis design



Forward: manufacturing innovations
- More efficient precursor
  Alkynes growth

- More sustainable resources
  Gaseous product mixture from Fischer-Tropsch synthesis
  Upcycling waste plastics
  Electrochemical conversion of $CO_2$

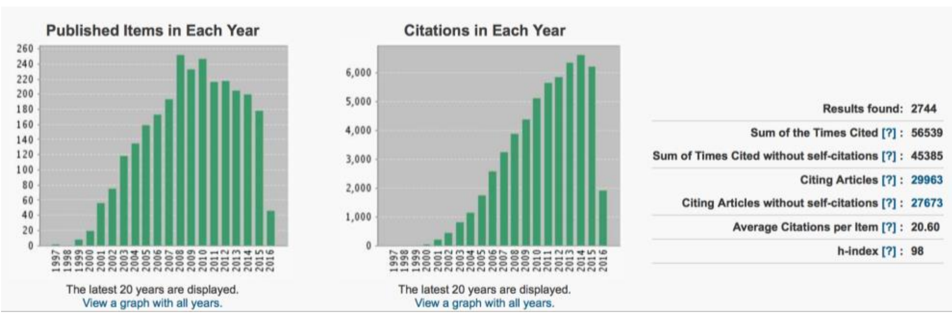
- Reactor modifications
  Continuous manufacturing
  Gas flow direction control
  Cold-walled reactor

# Data Extraction

## Chosen groups

Topic: “carbon nanotube” AND “growth” AND “chemical vapor deposition

Searched results: 2744



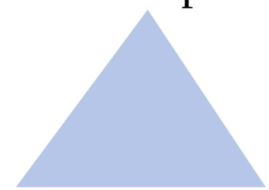

Ranked by record count

| View Records / Exclude Records | Field: Authors | Record Count | % of 2744 | Bar Chart |
|---|---|---|---|---|
| | ROBERTSON J | 53 | 1.931 % | |
| | ZHANG Q | 47 | 1.713 % | |
| | WEI F | 46 | 1.676 % | |
| | HOFMANN S | 36 | 1.312 % | |
| | HOMMA Y | 31 | 1.130 % | |
| | HART AJ | 30 | 1.093 % | |
| | HATA K | 29 | 1.057 % | |
| | MILNE WI | 29 | 1.057 % | |
| | AJAYAN PM | 28 | 1.020 % | |
| | HUANG JQ | 27 | 0.984 % | |
| | LEE JH | 23 | 0.838 % | |

ISI Web of Science database

## Collected parameters

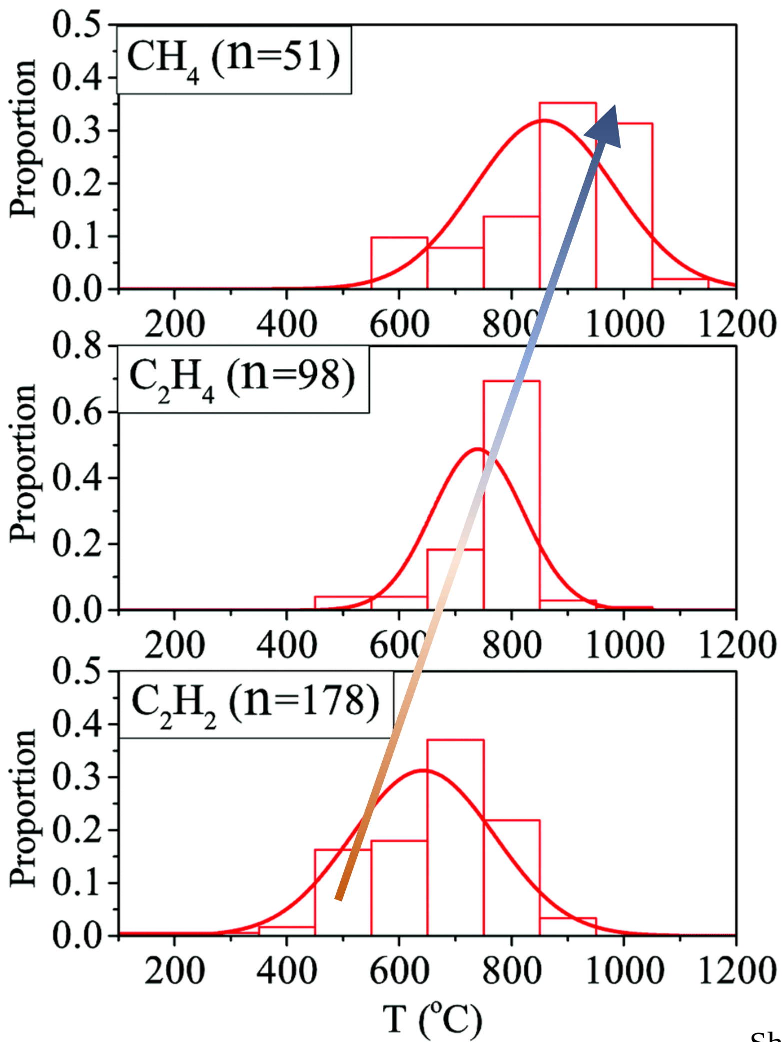
Energy
- Temperature



Resource
- $C_xH_y$ source
- $C_xH_y$ flow rate
- $H_2$ flow rate
- Carrier gas type
- Carrier gas flow rate
- Enhancer type
- Enhancer concentration
- Catalyst

Other
- Reactor type
- Reactor size

# Pattern 1: Temperature Dependence

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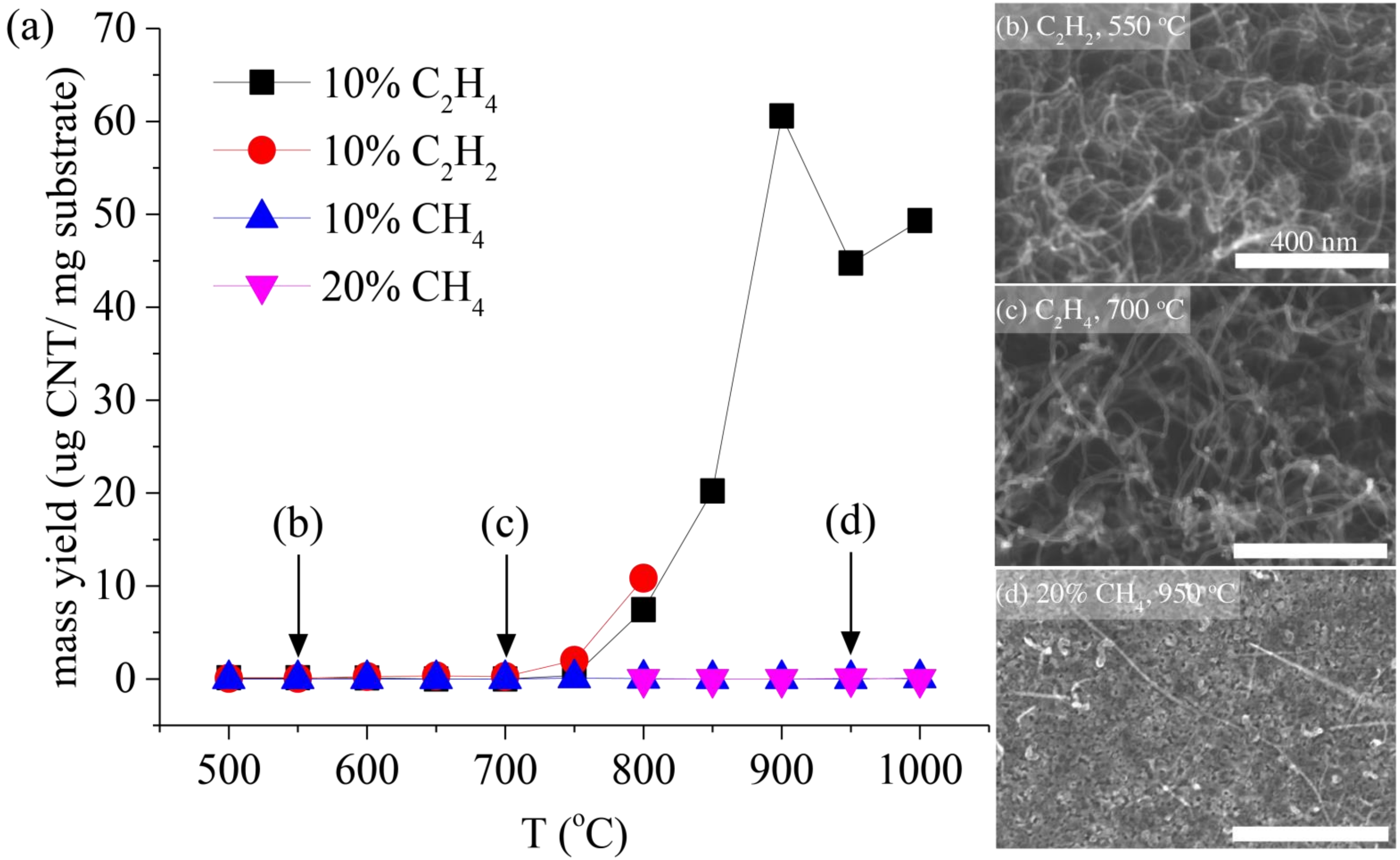
# Clarify Potential Biases: Experiments

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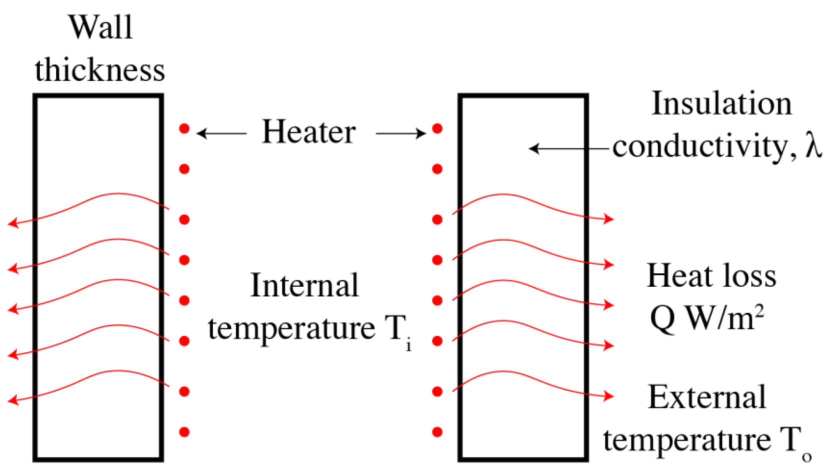
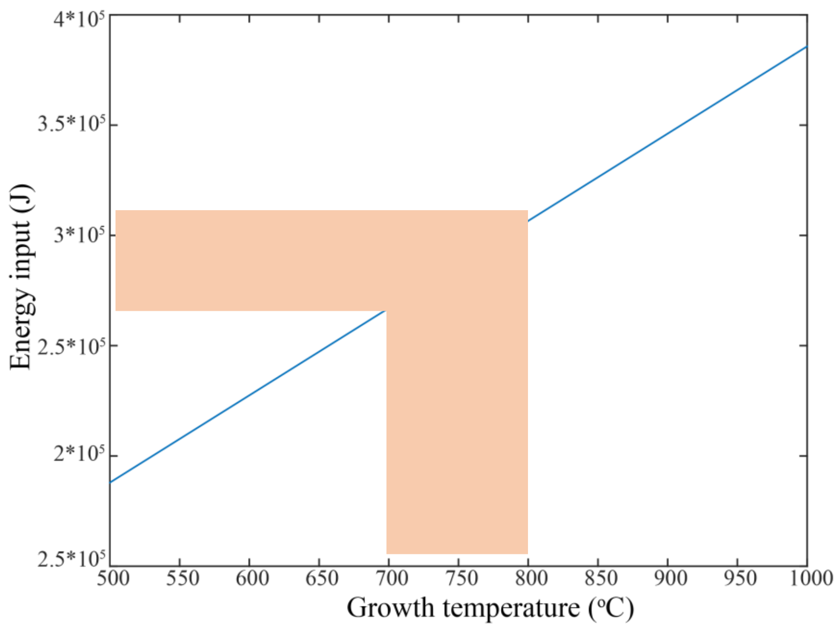
# Implication of Temperature Decrease

Thermal Loss Model




Energy saving: $1.3*10^{11}$ J/kg CNTs X Annual production: $2.2*10^{6}$ kg/year

$=2.9*10^{17}$ J/year ~ 7 million US household electricity consumption

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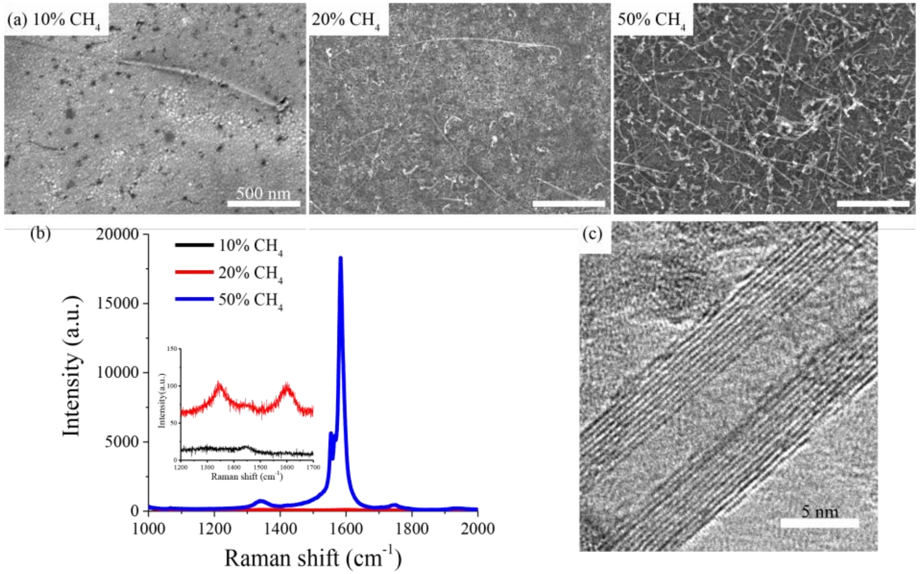
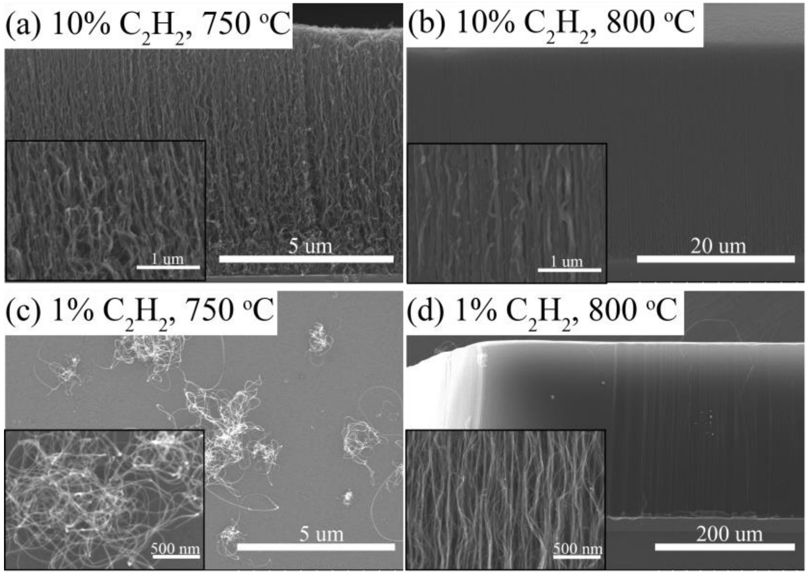
# Pattern 2:
# Material Demand: C and H loading

$CH_4$: high C loading




$C_2H_2$: low C loading

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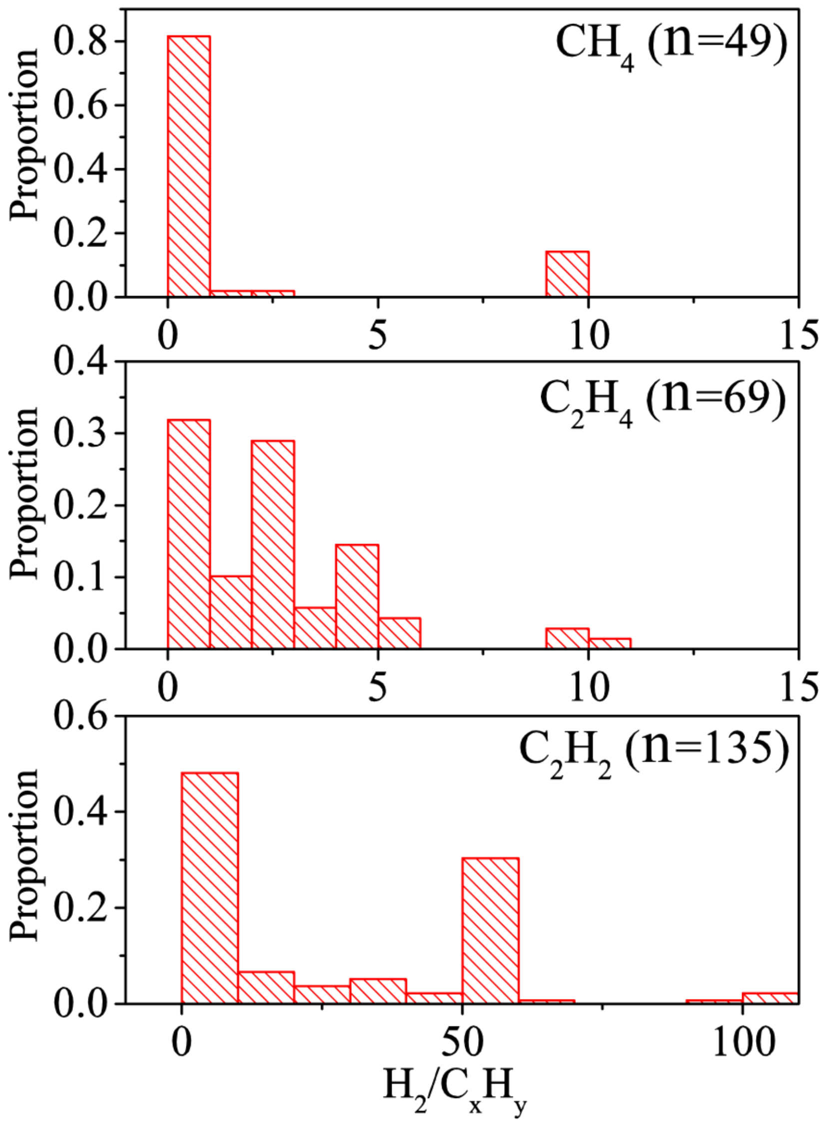
# Varied $H_2$ dependence

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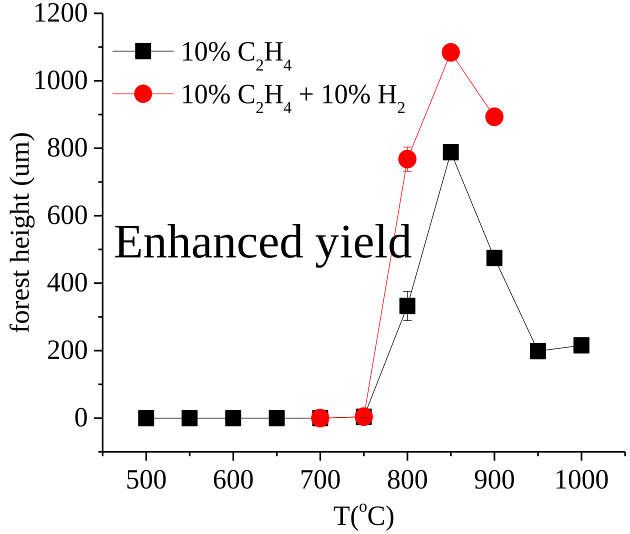
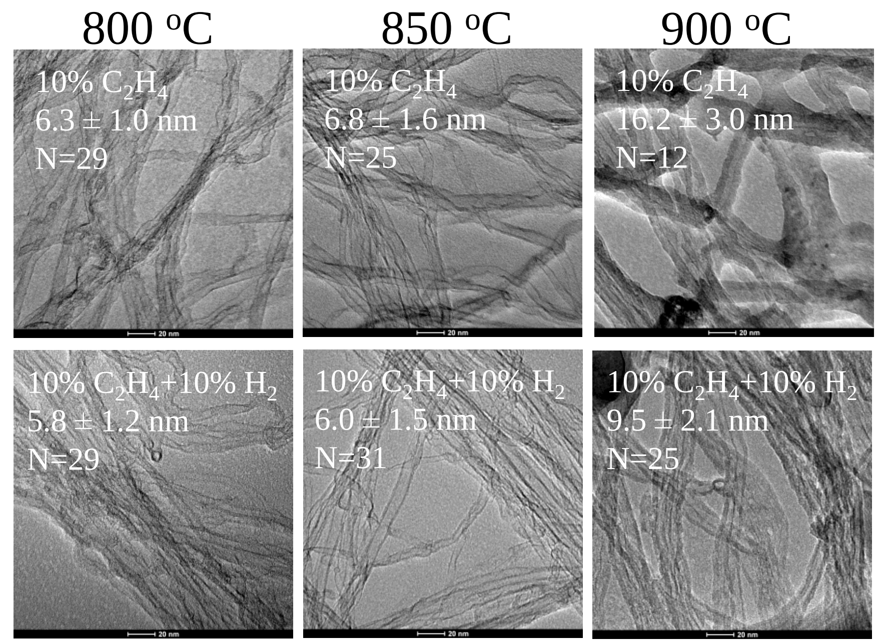
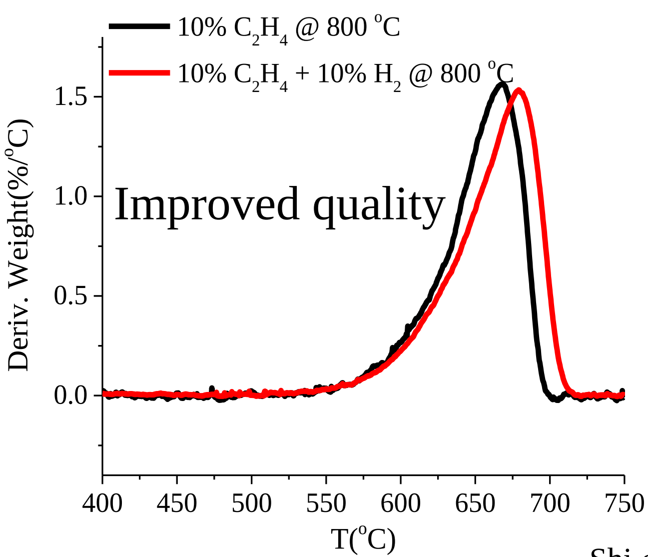
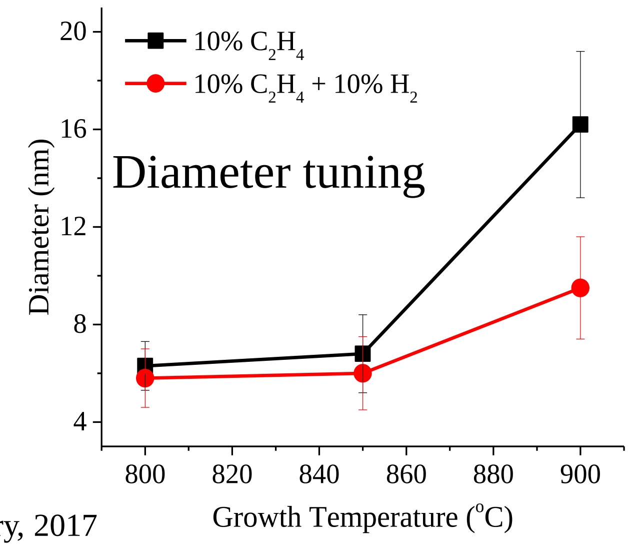
# Role of $H_2$

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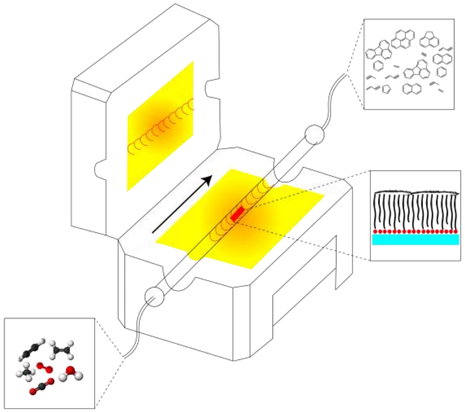
# Atom Carbon Efficiency

$$\text{Atomic Efficiency} = \frac{\text{C mass in CNT}}{\text{C mass in input precursor}}$$



| Growth Condition | Atomic Efficiency |
|---|---|
| Futaba et al. (Hata Group, 10% $C_2H_4$, 750 $^oC$) | 0.042% |
| Li et al. (Hart Group, 17% $C_2H_4$, 775 $^oC$) | 0.050% |
| Plata et al. (20% $C_2H_4$, 725 $^oC$, cold-wall reactor) | 0.002% |
| Plata et al. (Alkyne-assisted 20% $C_2H_4$, 725 $^oC$, cold-wall reactor) | 0.026% |
| 10% $C_2H_4$, 800 $^oC$ | 0.038% |
| 10% $C_2H_4$ + 10% $H_2$, 800 $^oC$ | 0.061% |
| 1% $C_2H_2$, 800 $^oC$ | 0.42% |

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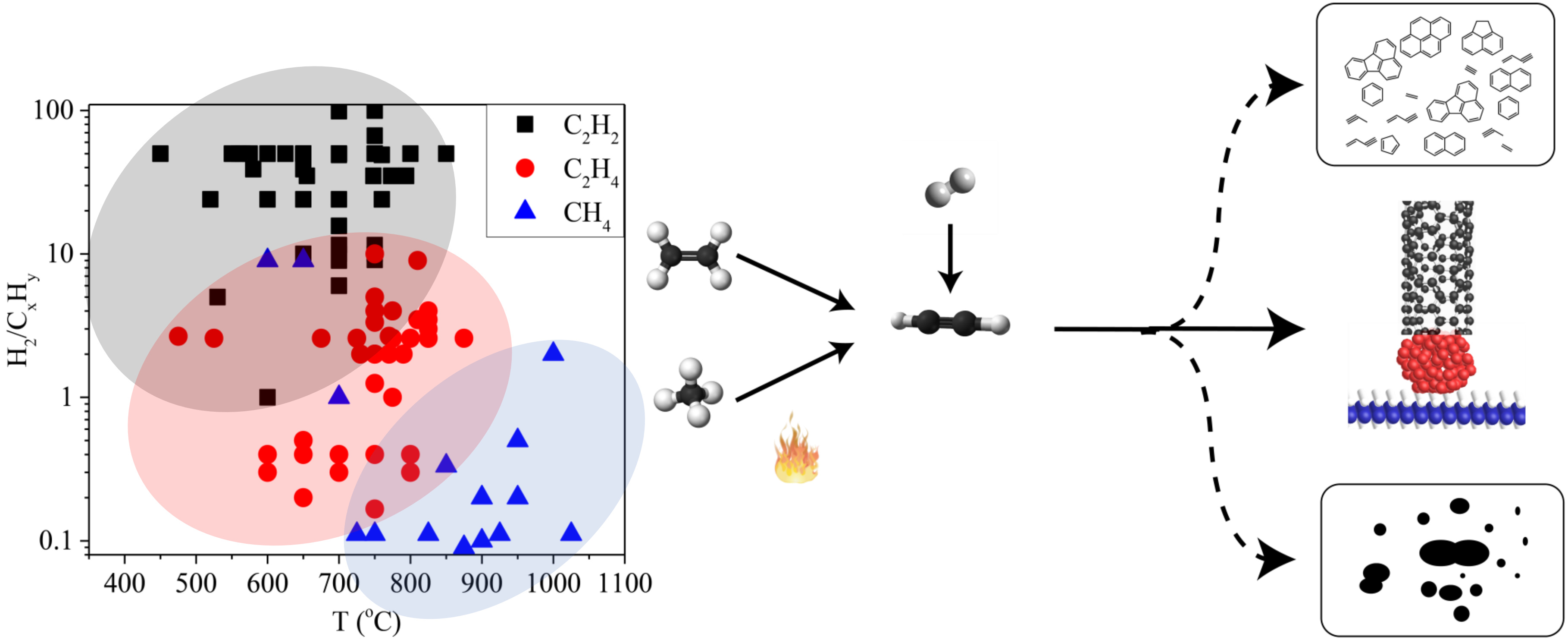
# Mechanistic Insights

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# Future Work

- Should be automated for high-throughput screening

- Methodology transferable to green synthesis of other novel materials

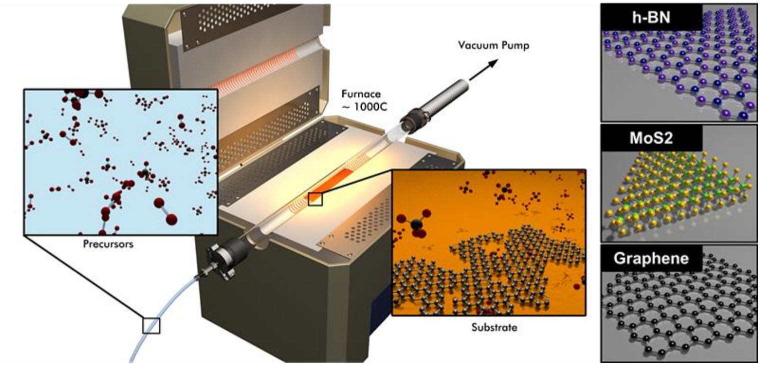


Image courtesy of Kong group at MIT

- Link product application performance to synthetic methodologies

Synthetic methodology → Product application performance

# Acknowledgements

ENGINEERS

BREADTH·DEPTH·PURPOSE

NSF

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

LC nano

# Temperature evolution