2D polymerization strategies: synthesis of graphdiyne film

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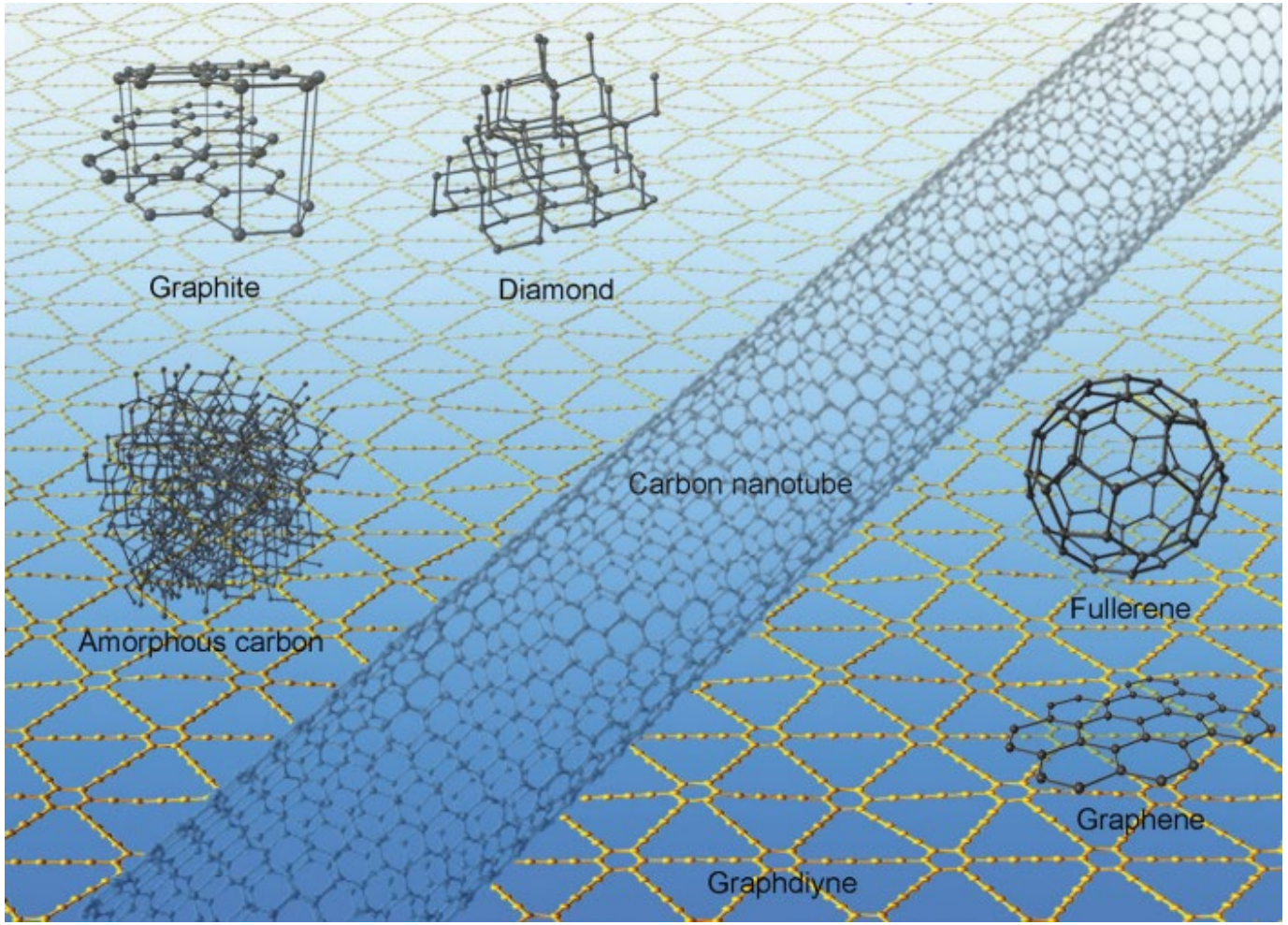
0. Content

1. Overview of Graphdiyne

1.1 Graphynes: structures

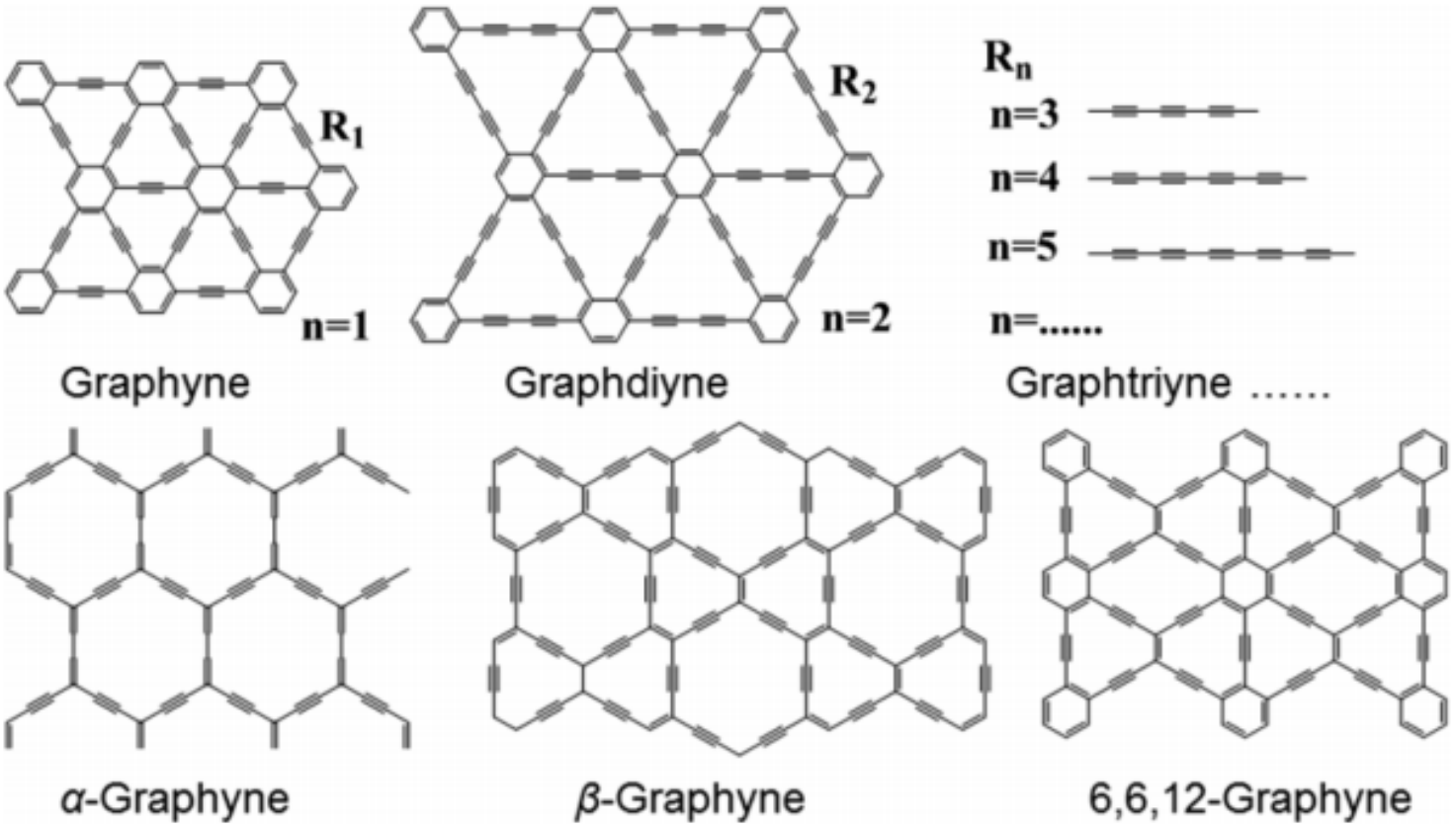


Chem. Commun. **2010**, 46, 3256-3258.

1. Overview of Graphdiyne

1.1 Graphynes: structures

GY **GDY**



Chem. Rev. **2018**, 118, 7744-7803.

1. Overview of Graphdiyne

1.2 GDY: properties & applications

2D porous material	
Properties:	**Applications:**
1. triangle pore side length: 3.8 Å	
- 3.8 Å < CH_4/CO - 3.8 Å > H_2O/H_2	1. gas absorption/separation
- 3.8 Å > metal ions	2. ion battery (ion passway)
2. sp π-bond:	
- metal coordination	3. catalysis carrier
- π-π interaction	
- inhibitive ability for free radical	4. radical scavenger
- hydrophobic	5. H_2O purification

Chem. Rev. **2018**, 118, 7744-7803.

1. Overview of Graphdiyne

1.2 GDY: properties & applications

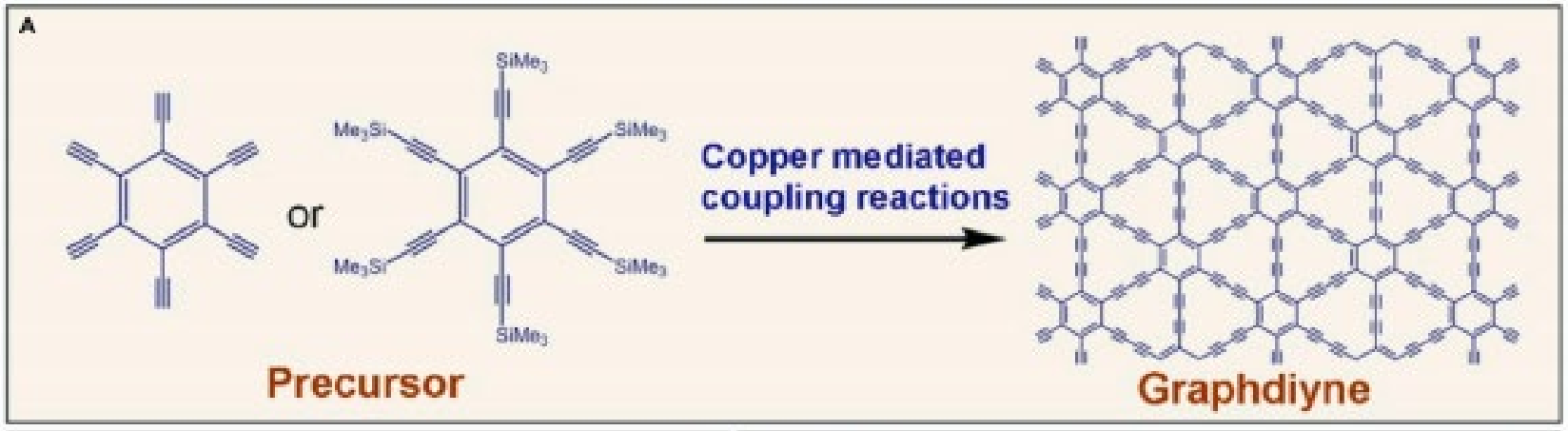
2D semiconductor	
Properties:	**Applications:**
1. bandgap: 0.44 – 1.47 eV 2. mobility: 10^4 $cm^2V^{-1}s^{-1}$ (DFT)	1. electronic device 2. photosensor 3. vapor detector
3. high photothermal conversion efficiency	4. photothermal therapy (PTT)

Chem. Rev. **2018**, 118, 7744-7803.

1. Overview of Graphdiyne

1.3 GDY: synthesis

The only strategy: solution-phase synthesis

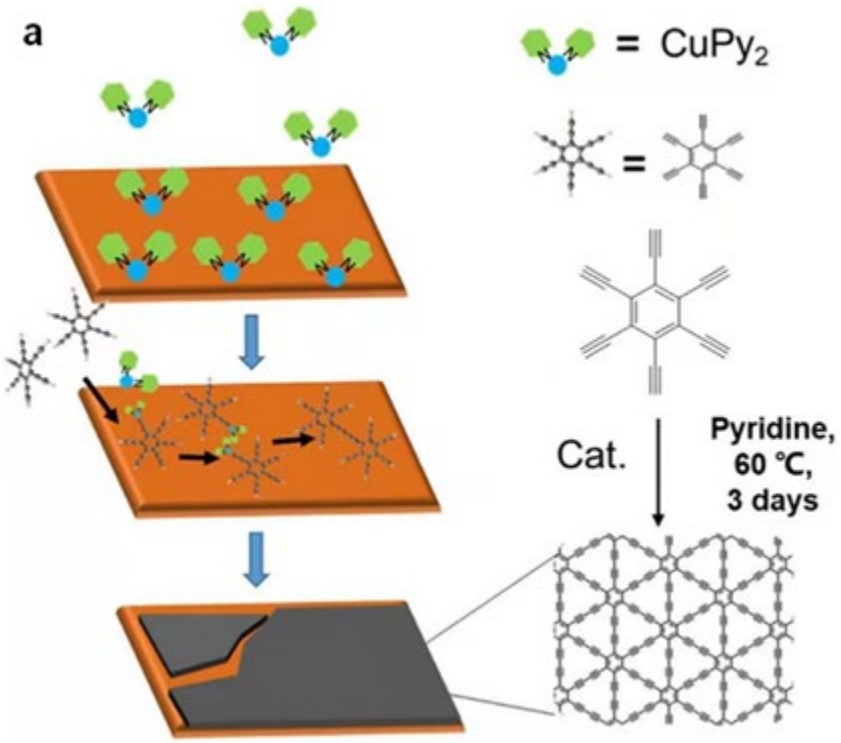


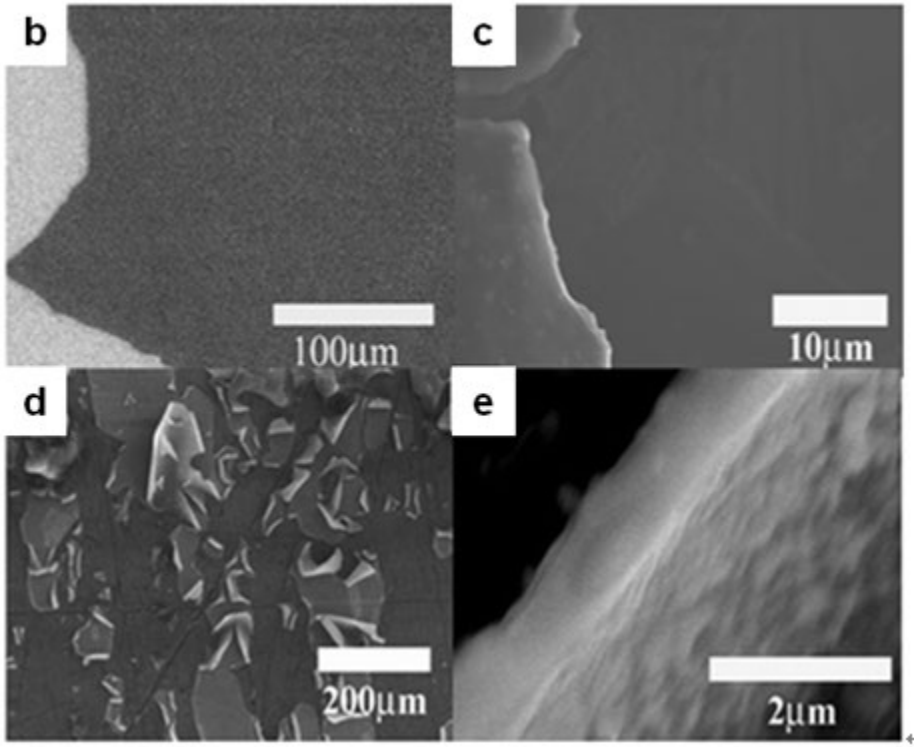
hexaethynylbenzene (HEB)

Chem **2020**, 6, 1-19.

1. Overview of Graphdiyne

1.3 GDY: synthesis





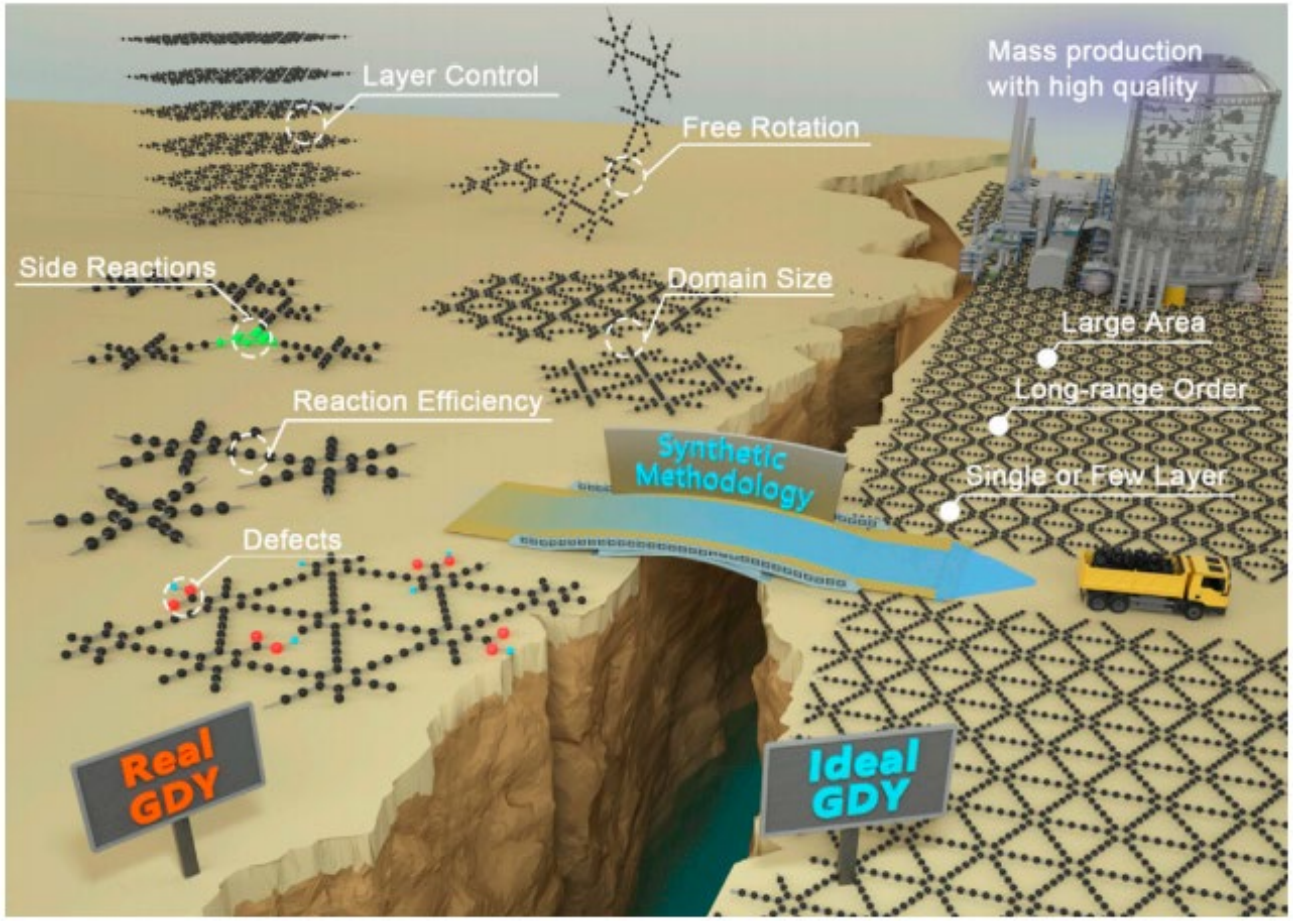
Cu is oxidized to Cu ions in a basic solvent

Chem. Commun. **2010**, 46, 3256-3258.

1. Overview of Graphdiyne

1.4 From real to ideal GDY film

1. High quality 2. μm^2 area 3. Layer control 4. Easy to transfer



Chem **2020**, 6, 1-19.

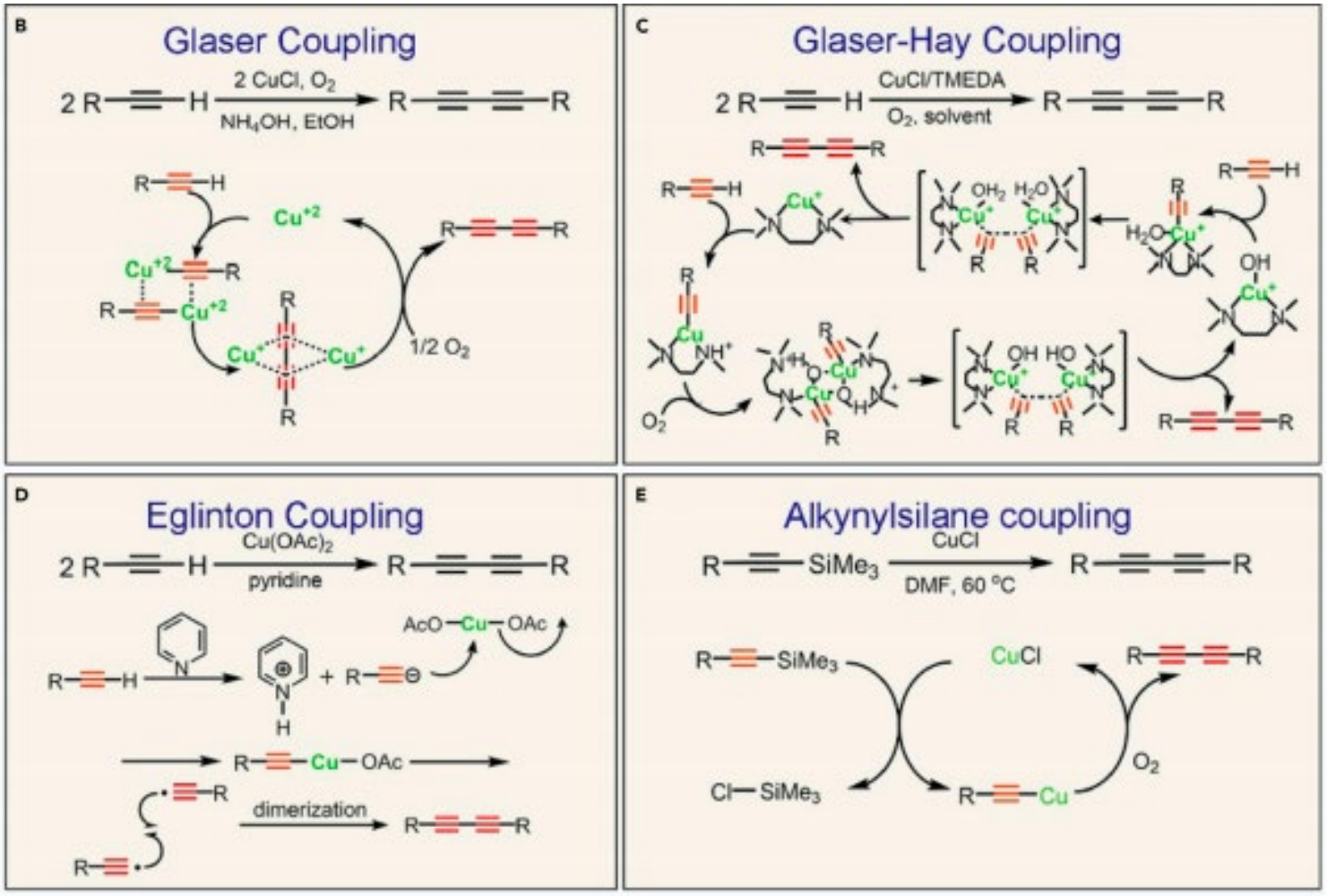
1. Overview of Graphdiyne

1.4 From real to ideal GDY film

Ideal GDY film	Synthesis strategies
Microscopic:	**Microscopic:**
1. High quality - side reaction/defect (selectivity) - domain size (nucleation site)	2.1 new reaction mechanism
- relative rotation	2.2 monomer-substrate alignment effect
Macroscopic:	**Macroscopic:**
2. μm^2 area	3 flat & confined 2D reaction interface: spatial distribution of
3. Layer control	3.1 catalyst 3.2 monomer 3.3 temperature
4. Easy to transfer (compared with Cu)	

2. Microscopic control

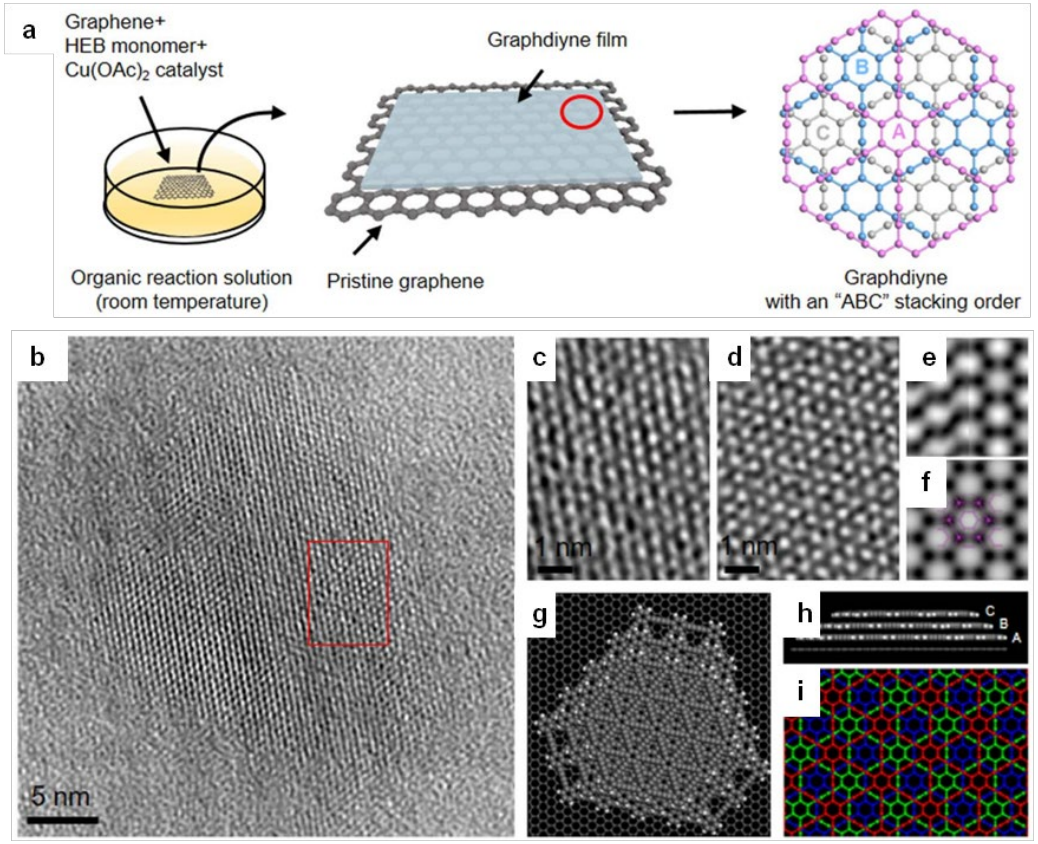
2.1 New reaction mechanism



Chem **2020**, 6, 1-19.

2. Microscopic control

2.2 Monomer-substrate alignment effect



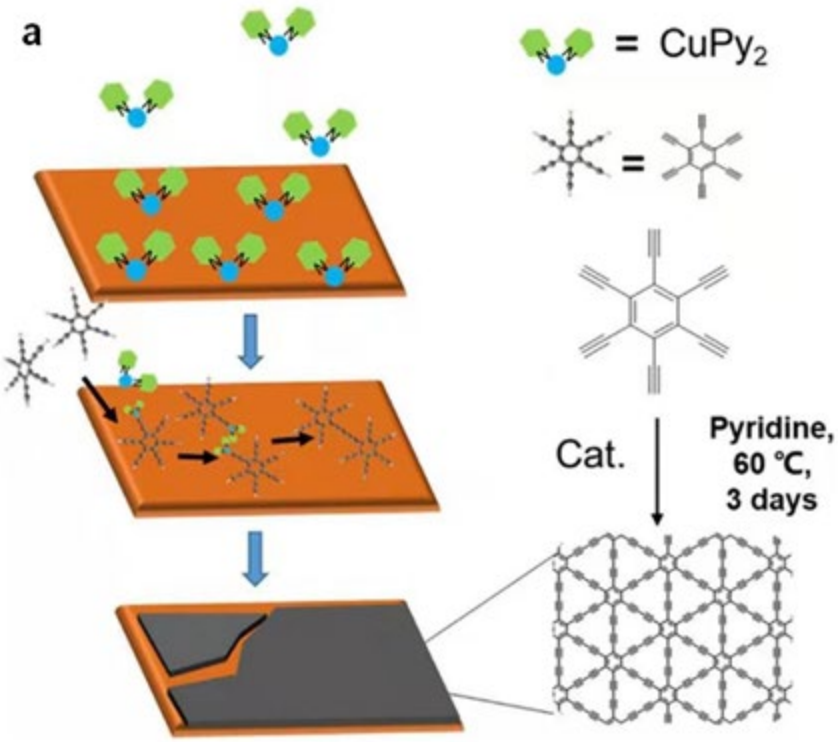
1. high quality
2. triple-layer

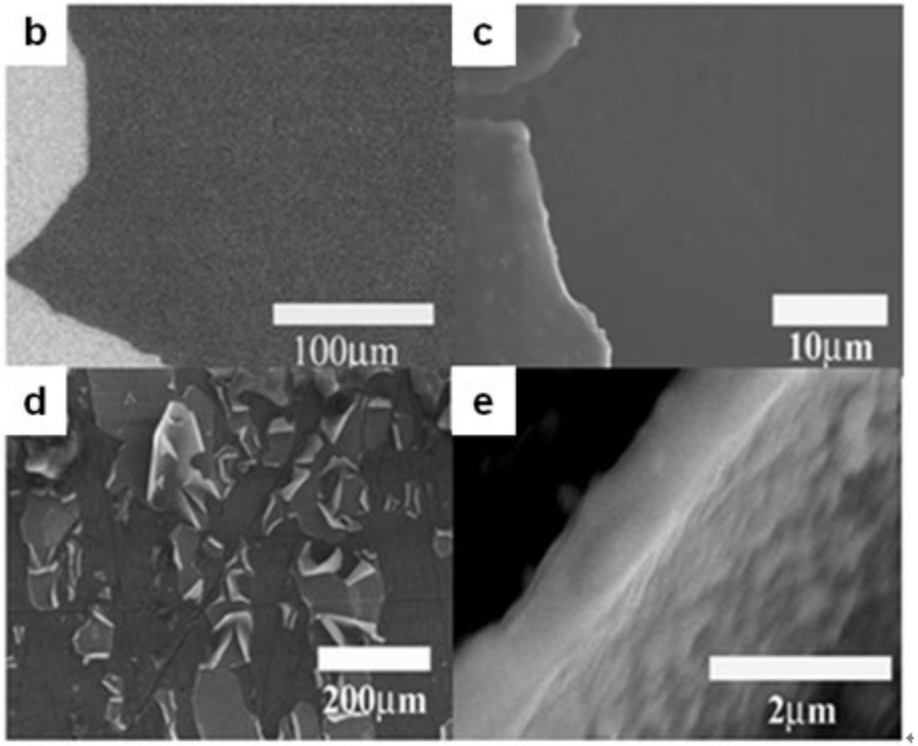
1. hard to transfer
2. area: too small

Sci. Adv. **2018**, 4, eaat6378.

3. Macroscopic control

3.1 Confined 2D spatial distribution of catalyst





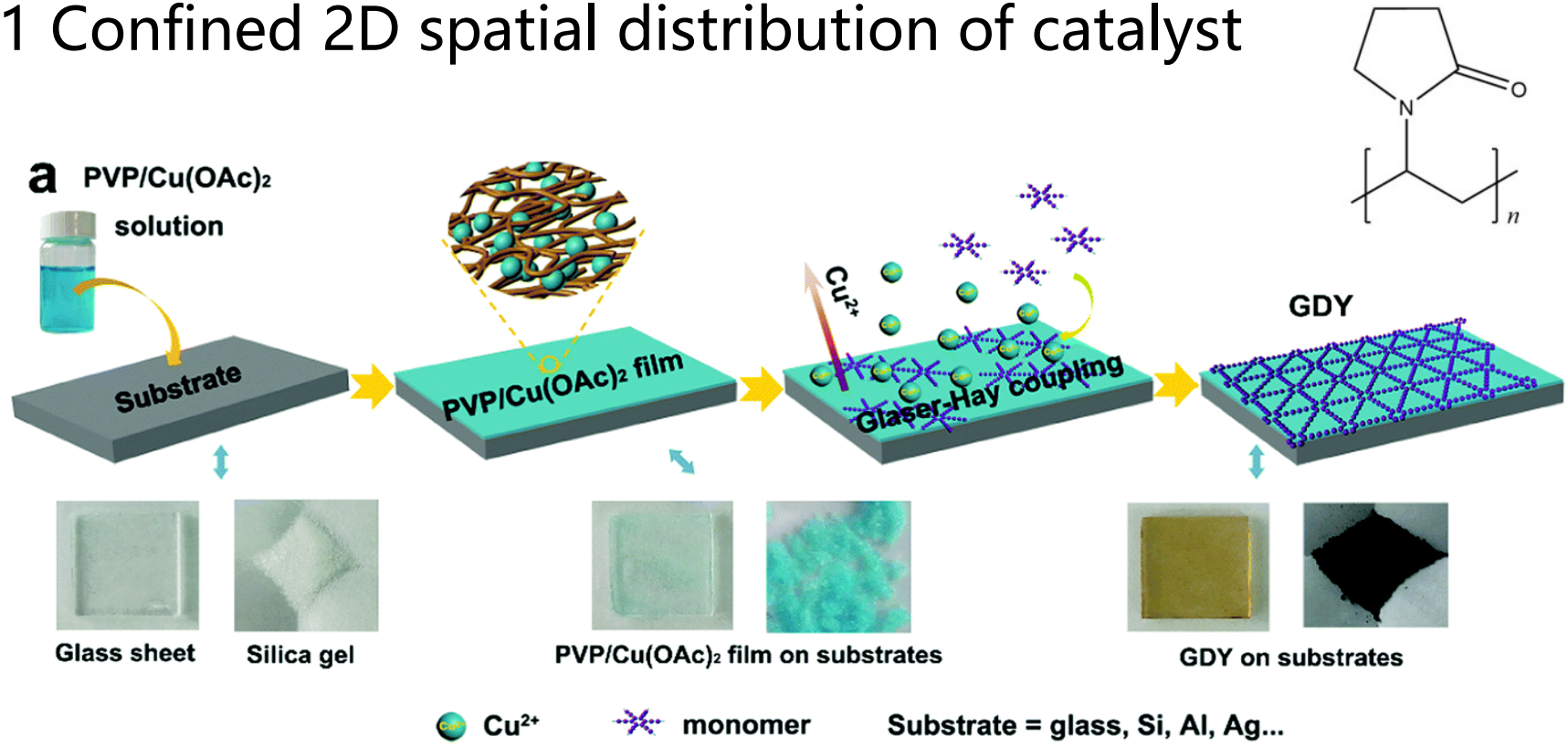
1. μm^2 area

1. random layer number

Chem. Commun. **2010**, 46, 3256-3258.

3. Macroscopic control

3.1 Confined 2D spatial distribution of catalyst



1. controllable [Cu^{2+}]
2. arbitrary substrate

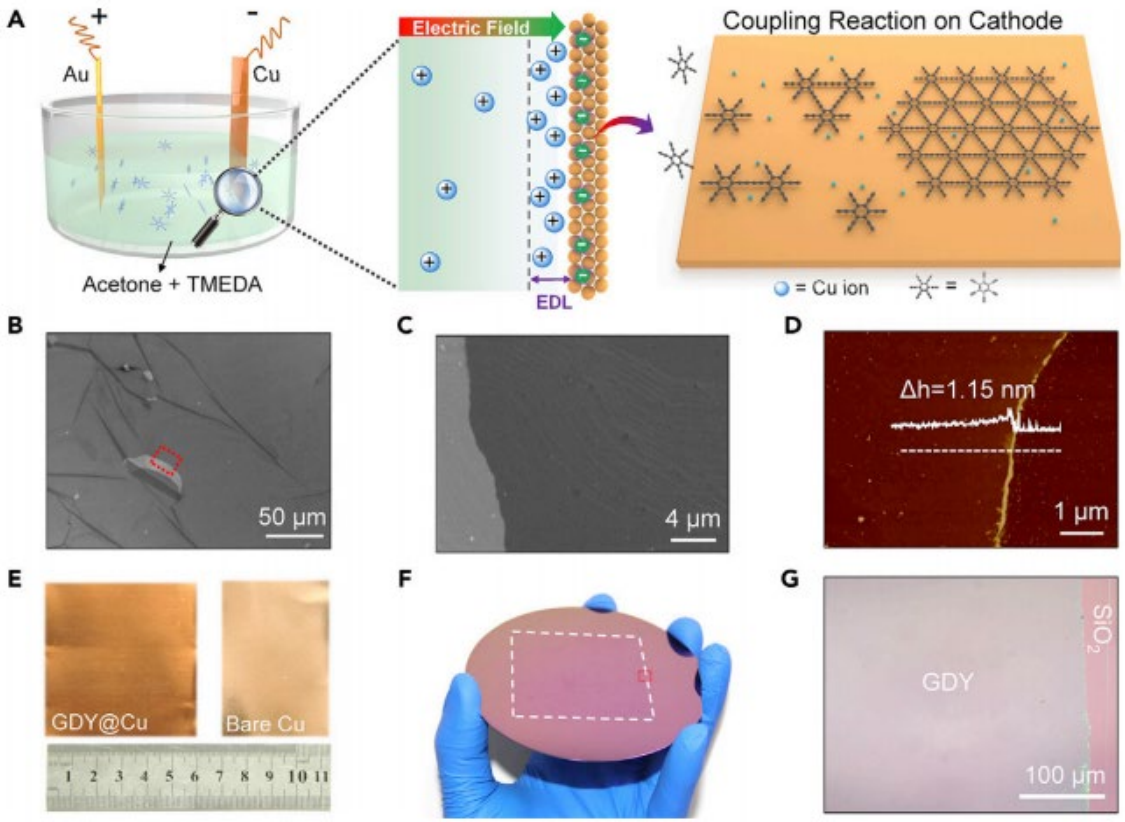
0. not flat
1. area: too small
2. random layer number

Chem. Commun. **2018**, 54, 6004-6007.

3. Macroscopic control

3.1 Confined 2D spatial distribution of catalyst

Cu ions release from Cu foil (not because of electrochemical reaction)



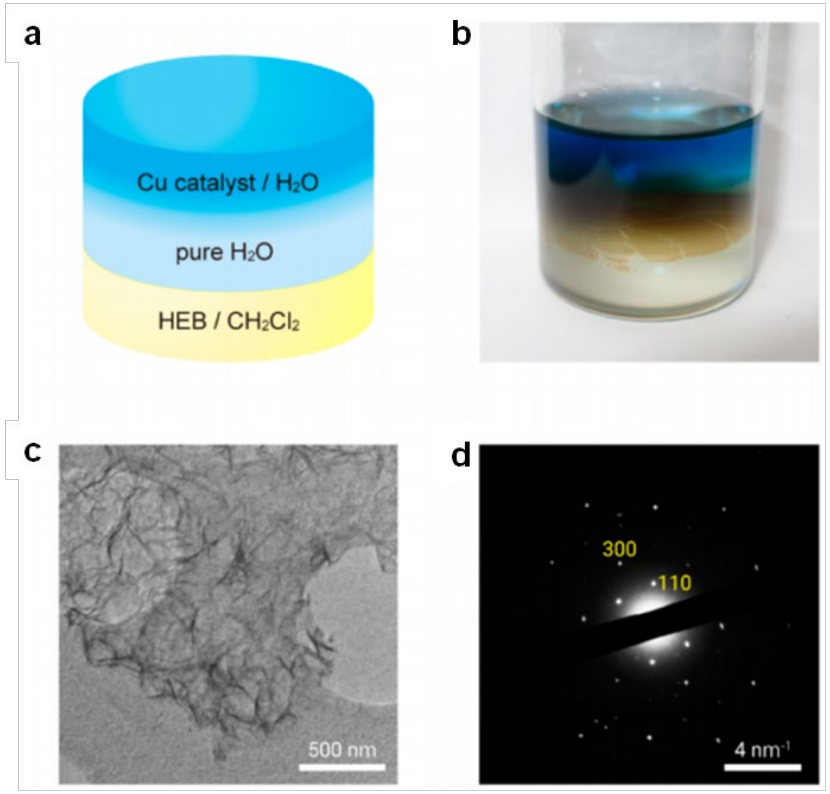
electric double layer (EDL)

1. triple-layer
2. wafer-scale area

Chem **2021**, 7, 1-13.

3. Macroscopic control

3.2 Confined 2D spatial distribution of catalyst & monomer



liquid-liquid interface:
unstable &
interdiffusion layer

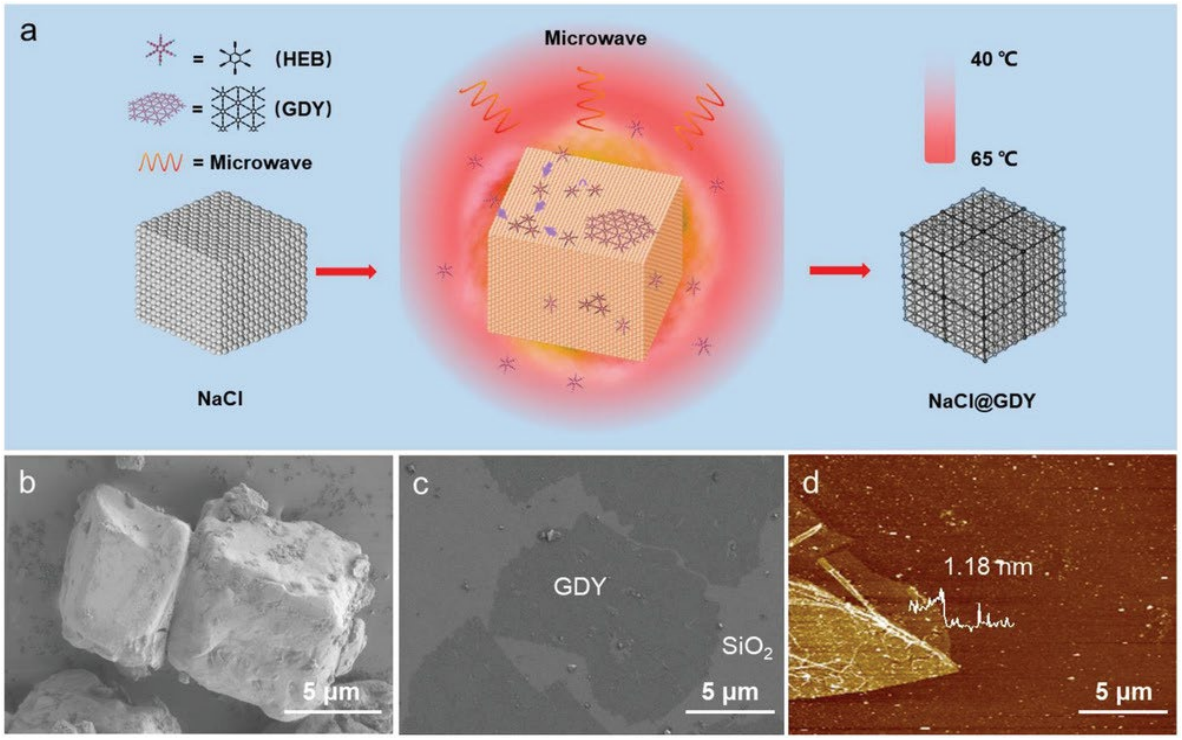
1. easy to transfer

1. poor quality
2. area: too small
3. random layer number

J. Am. Chem. Soc. **2017**, 139, 3145– 3152.

3. Macroscopic control

3.3 Confined 2D spatial distribution of temperature



1. triple-layer
2. μm^2 area
3. easy to transfer
4. cat. free

Adv. Funct. Mater. **2020**, 30 20011396.

4. Conclusion

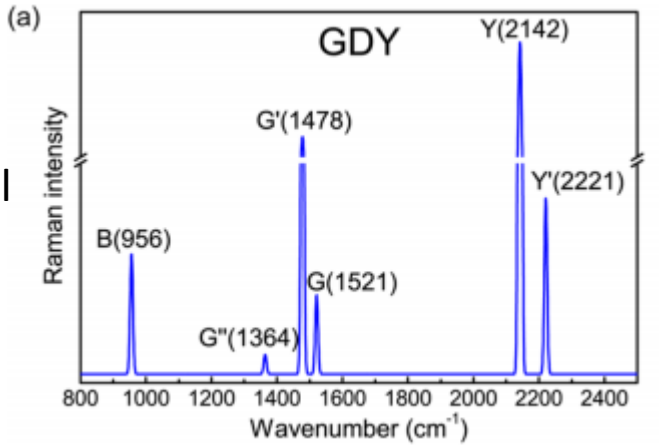
4.1 Prototype for 2D polymerization strategies

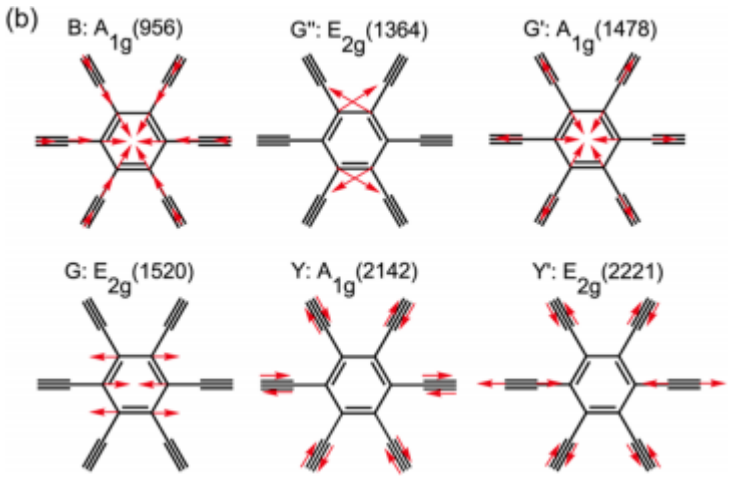
Ideal GDY film	Synthesis strategies
Microscopic:	**Microscopic:**
1. High quality - side reaction/defect (selectivity) - domain size (nucleation site)	2.1 new reaction mechanism
- relative rotation	2.2 monomer-substrate alignment effect
Macroscopic:	**Macroscopic:**
2. μm^2 area 3. Layer control	3 flat & confined 2D reaction interface: spatial distribution of 3.1 catalyst 3.2 monomer 3.3 temperature
4. Easy to transfer (compared with Cu)	

4. Conclusion

4.2 Problems: poor quality

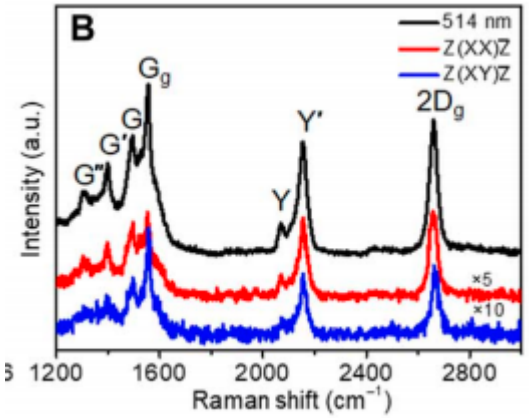
theoretical





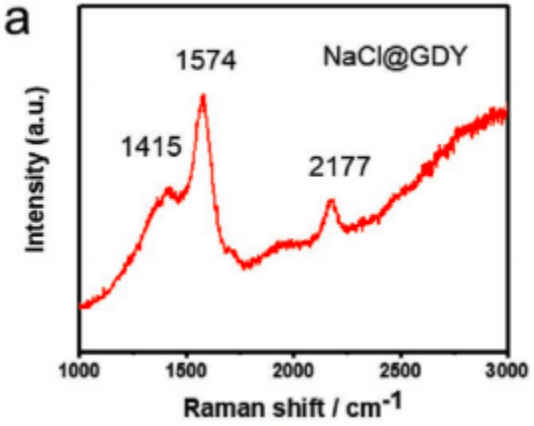
J. Phys. Chem. C **2016**, 120, 10605-10613.

Graphene alignment (3L)



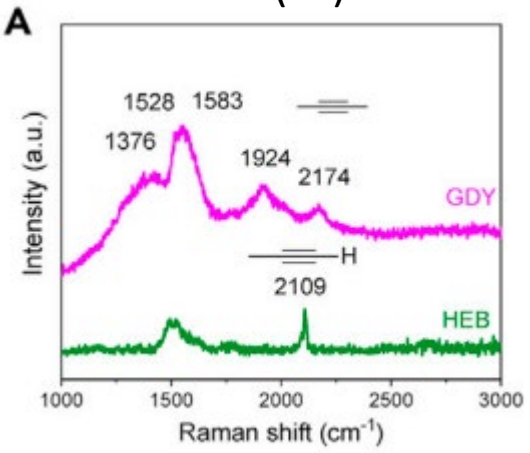
Sci. Adv. **2018**, 4, eaat6378.

NaCl microwave (3L)



Adv. Funct. Mater. **2020**, 30 20011396.

EDL (3L)



Chem **2021**, 7, 1-13.

Thanks