國立臺灣大學
應用力學研究所
National Taiwan University

Chemical Engineering Master Thesis Review:
以紫外光交聯之複合式生物墨水包覆人類脂肪幹細胞於生醫組織工程的應用

Computational Mechanics and Intelligence Lab
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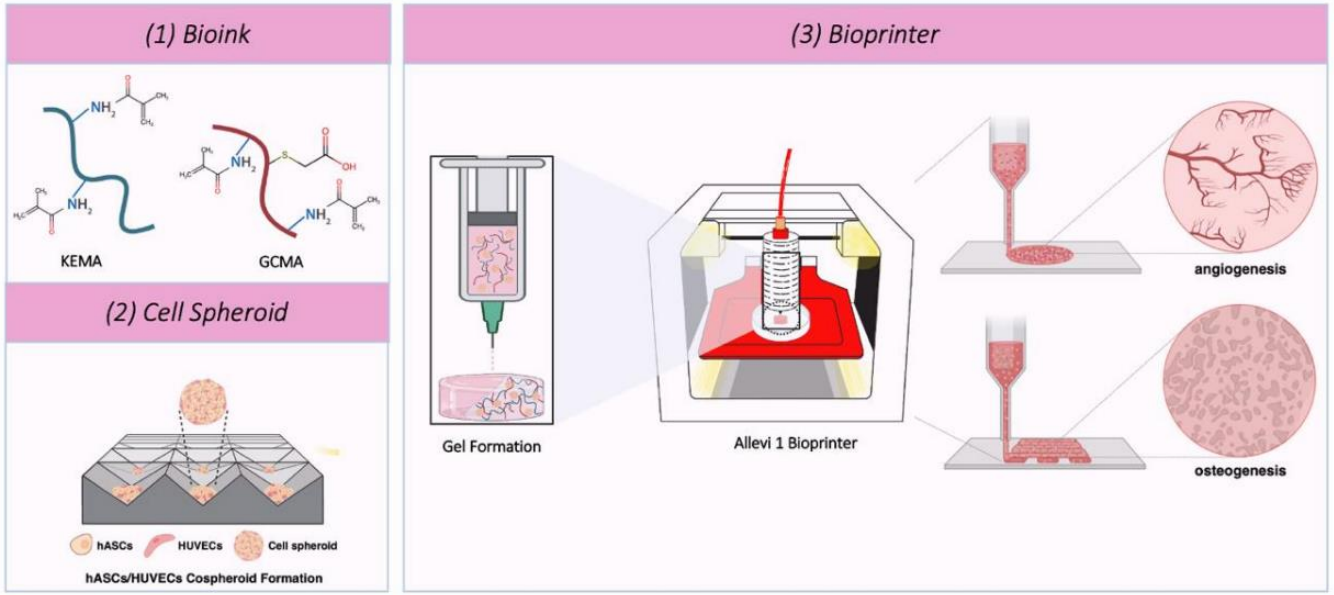
Reporter: Yu-Cheng Lai, Advisor: Chia-Ching Chou
Institute of Applied Mechanics, National Taiwan University
Stevenlai1998@gmail.com/ccchou@iam.ntu.edu.tw

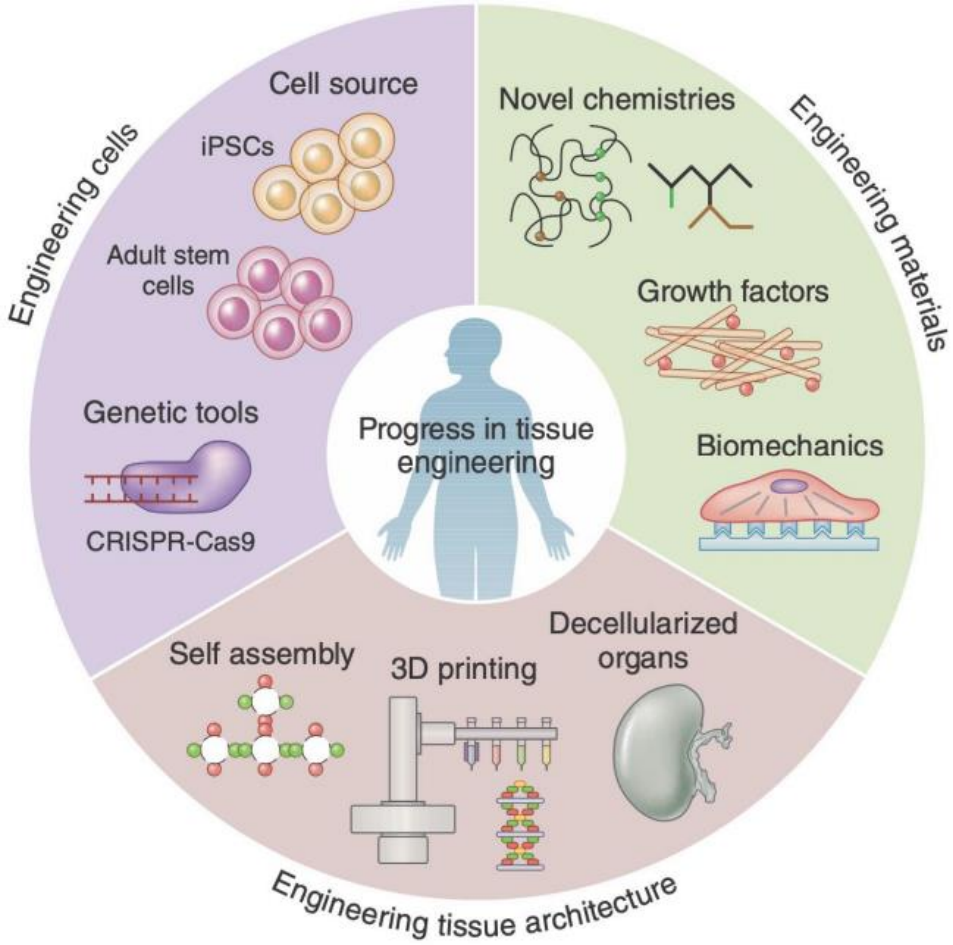
大綱

- 最後要做到的結果：github.com/nivation/KEMA-GCMA-hydrogel
- 論文簡介(20 min)
- 論文與模擬的關係(20 min)
- 回答問題(20 min)

Introduction (P1-P19)

- Tissue engineering-**material** to architecture
- 3D bioprinting and biolink
- Mechanical properties

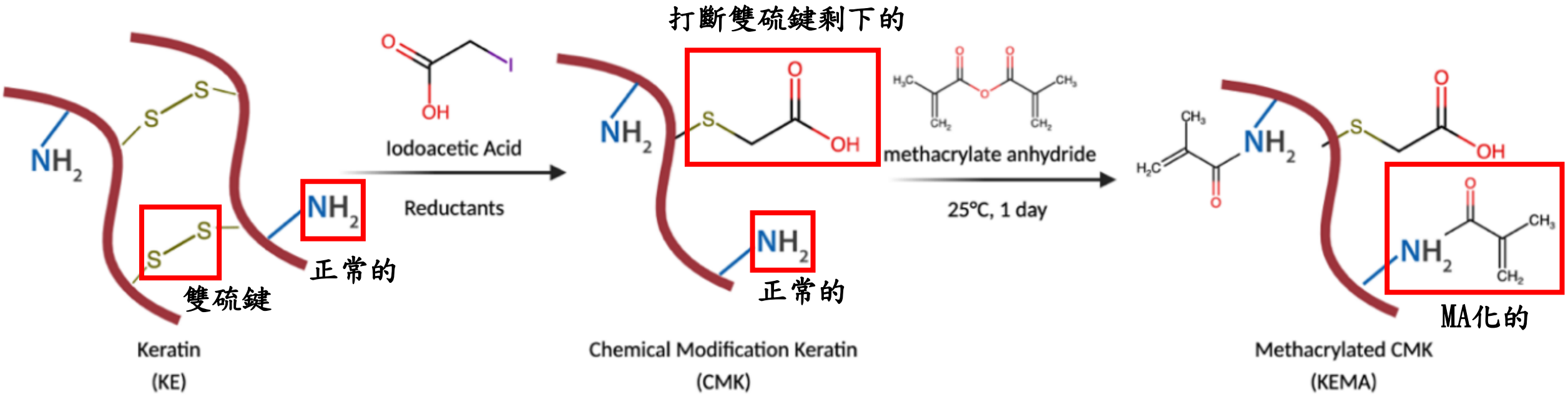




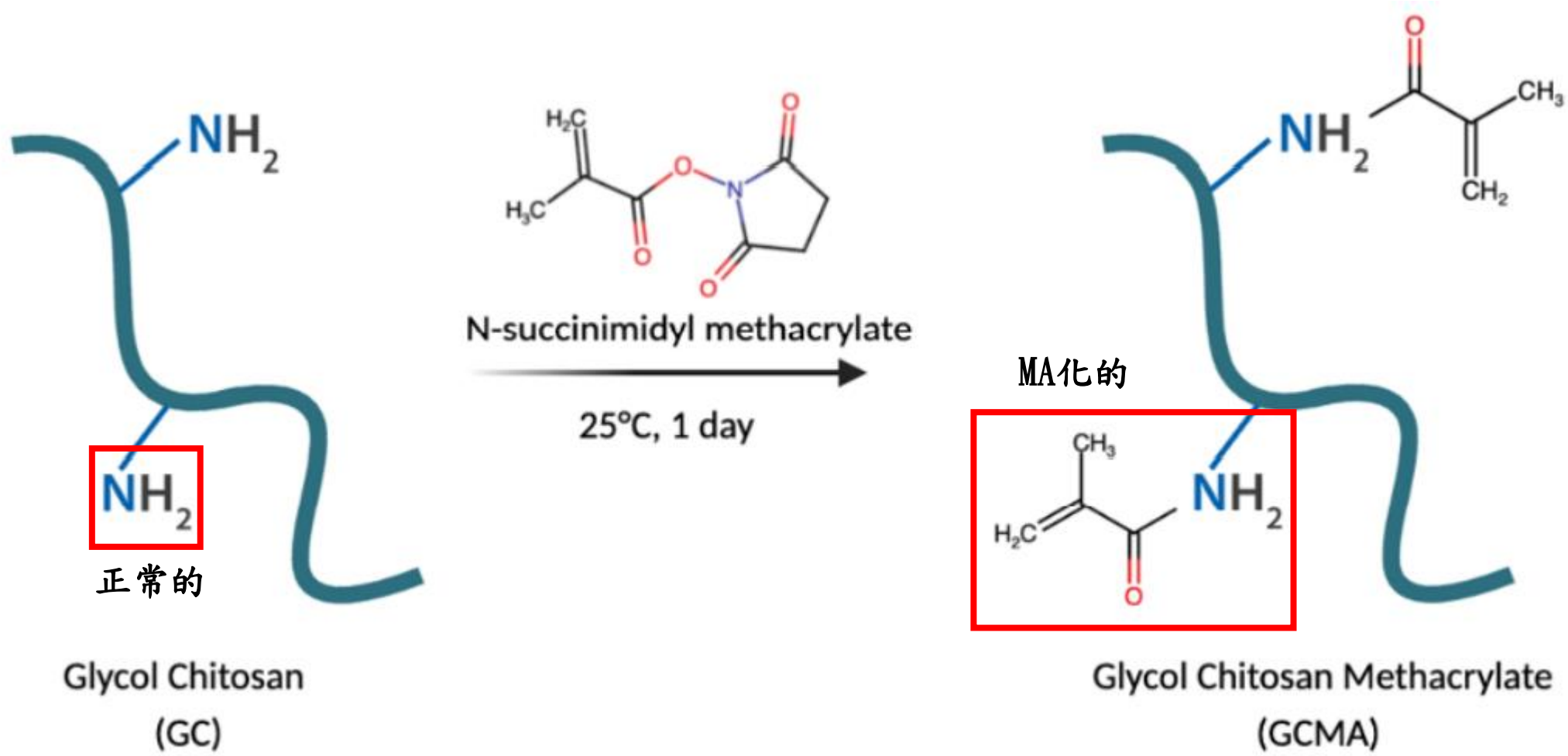
Materials and Methods (P29-31)

- 4 Materials for bio-ink
  - Glycol Chitosan > Methacrylated Glycol Chitosan (**GCMA**): **Hard** and strong
  - Keratin >斷雙硫鍵> Methacrylated keratin (**KEMA**): **Soft** and yummy
  - PBS solution: Prevent variation in PH value
  - photoinitiator: Enable polymerization

Keratin >斷雙硫鍵> Methacrylated keratin (KEMA)



Glycol Chitosan > Methacrylated Glycol Chitosan (GCMA)



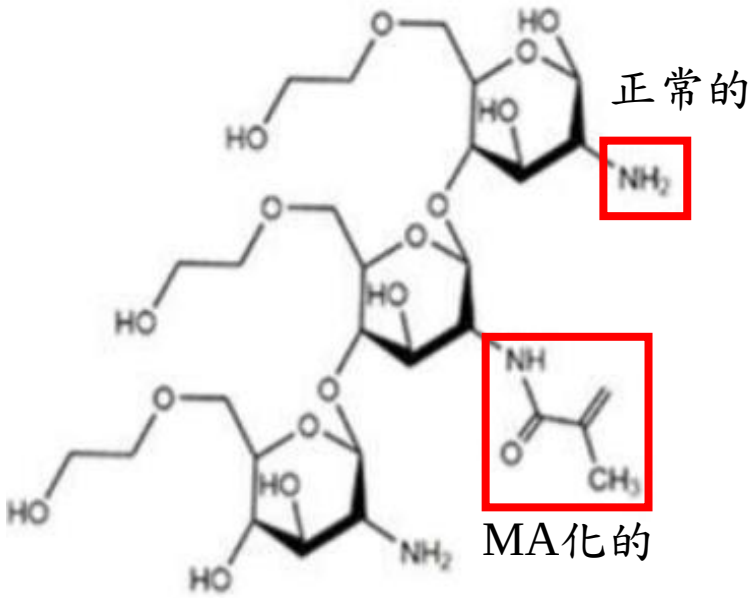
PBS Buffer Solution: Phosphate Buffered Saline

- 磷酸鹽緩衝生理鹽水
- Concentration of 1L PBS solution (PH=7.4)

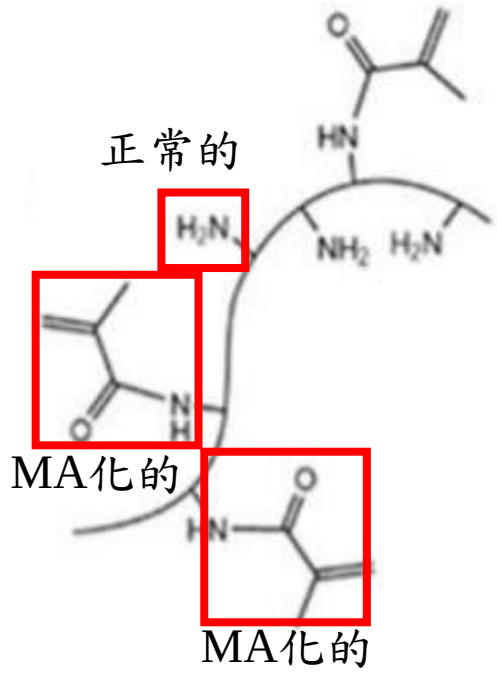
Salt	Effect	Gram (g)
NaCl	模擬人體	8
Na2HPO4	Buffer with HPO4	1.44
KCl	模擬人體	0.2
KH2PO4	Buffer with H2PO4	0.24

Materials and Methods

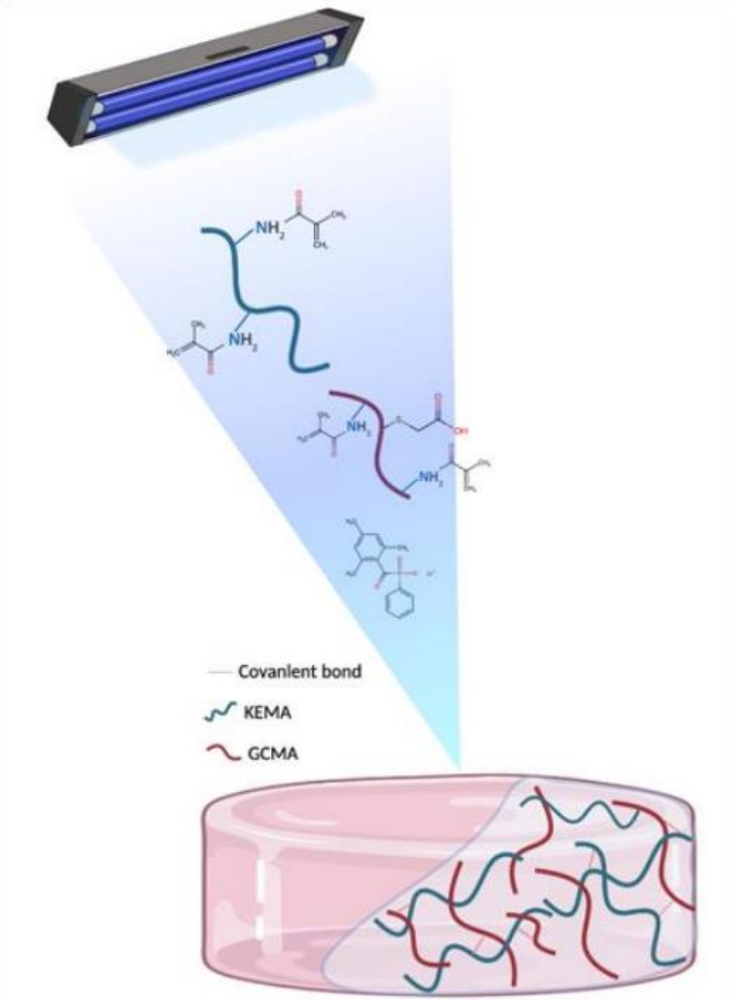
- Methods
  - UV-crosslinking: MA之間聚合



GCMA

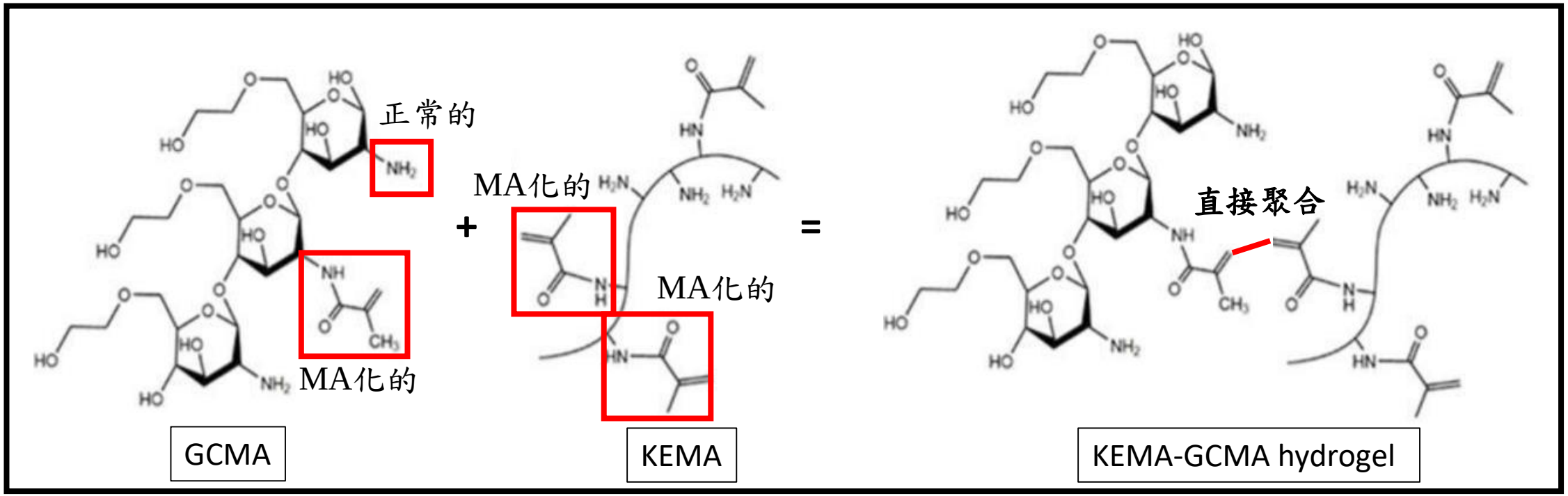


KEMA



Methacrylated and its polymerization (聚合反應)

1. 聚合以後，有沒有任何原子被丟掉了?
2. 聚合時，有沒有少任何原子?
3. 模擬上：少了甚麼關鍵的條件?



Experiment Design (P32.33) and Result (P43)

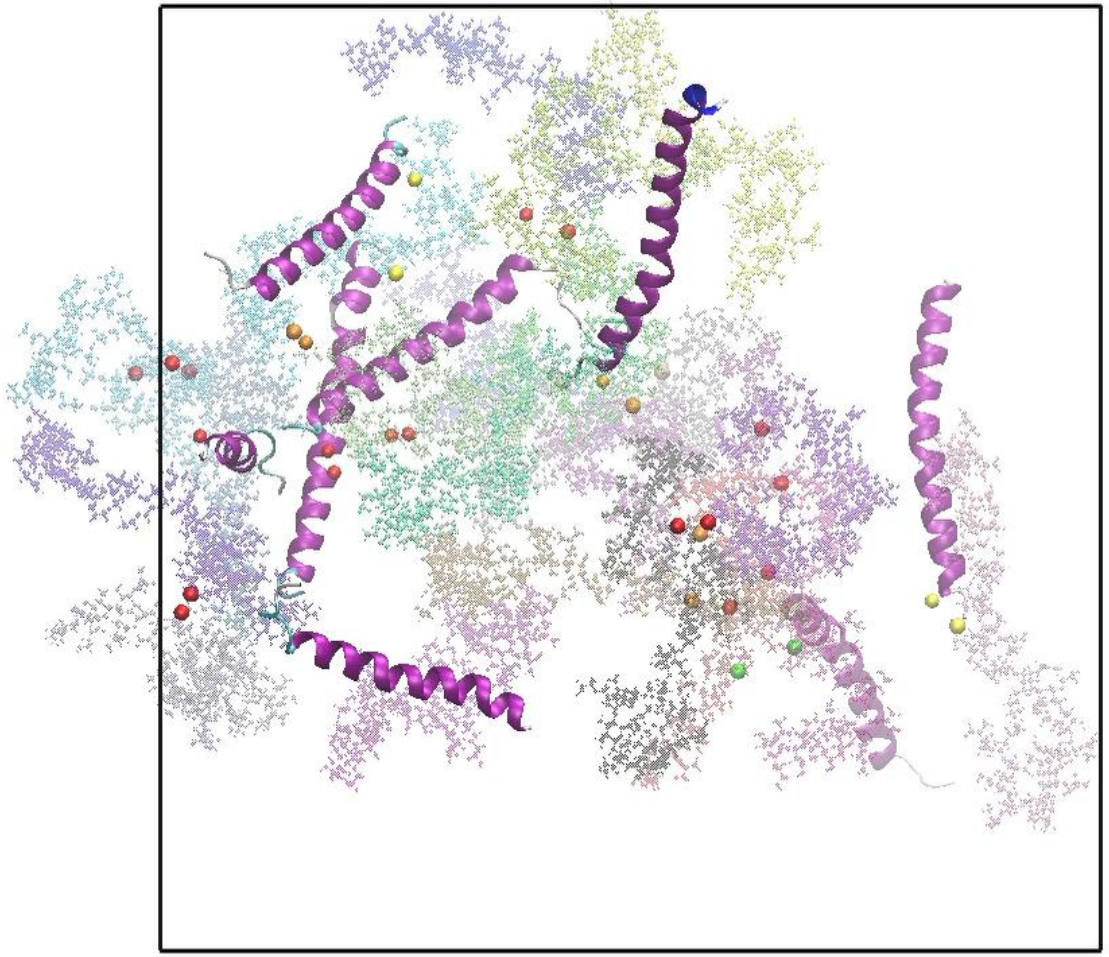
Model	water(g or ml)	KEMA(g)	GCMA(g)	NaCl(g)	Result
4% KEMA	100	4	0	0.8	最軟
4% GCMA	100	0	4	0.8	最硬
1%KEMA 3%GCMA	100	1	3	0.8	中

為甚麼要模擬&模擬如何和實驗溝通

- 為甚麼會變軟？角蛋白具體上怎麼影響了這個材料？
- 角蛋白很大，是每個部份的角蛋白都一樣重要嗎？還是只需要部份就可以了？
- 聚合是誰和誰聚合了？聚合的機率高嗎？聚合完對結構發生甚麼影響了？
- 未來，我們要如何建議實驗方調整他們的配比呢？最省錢？最硬？延展性最好？
- 實驗方憑甚麼相信我們？

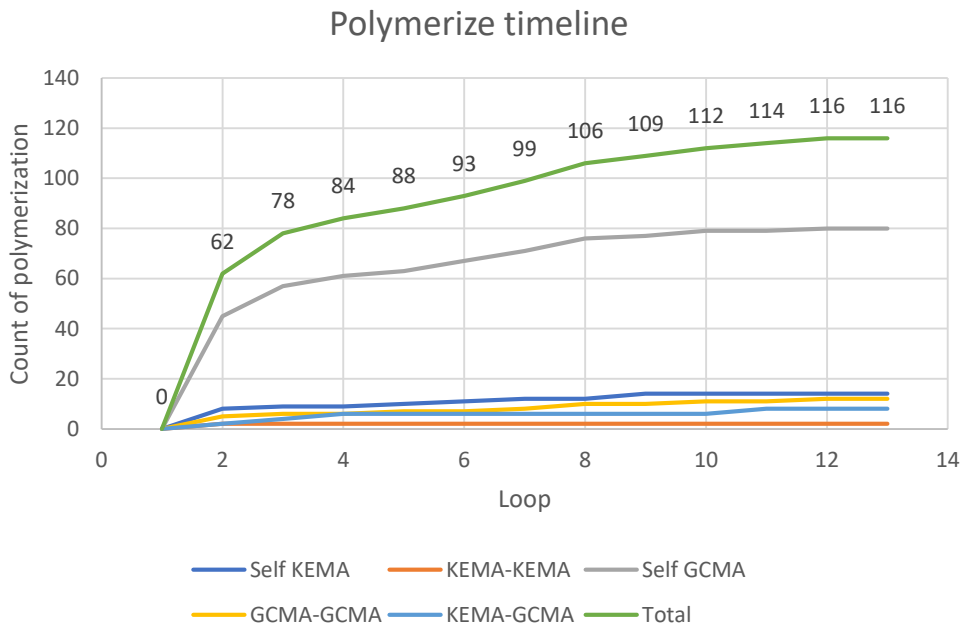
Setup and Simulation

- MD setup：
  - CPU: 160
  - Atom num: 326588
  - Pair Style: lj/charmmfsw/coul/long
  - Cmap: yes
  - Ensemble: **NPT temp 300 iso 1**
  - Timestep: 1 fs
  - Cost time: **0.1 ns / 3hr**



Simulation

- Polymerization percentage=$\frac{Polymerized\ Pair}{Modified\ MA\ number \div 2}$ =**62%**
- Major contribution of polymerization happens in **intra-GCMA**



loop	Self KEMA	KEMA-KEMA	Self GCMA	GCMA-GCMA	KEMA-GCMA	Total
1	0	0	0	0	0	0
2	8	2	45	5	2	62
3	9	2	57	6	4	78
4	9	2	61	6	6	84
5	10	2	63	7	6	88
6	11	2	67	7	6	93
7	12	2	71	8	6	99
8	12	2	76	10	6	106
9	14	2	77	10	6	109
10	14	2	79	11	6	112
11	14	2	79	11	8	114
12	14	2	80	12	8	116
13	14	2	80	12	8	116 (62%)

Answering following questions

(1)他們想幹嘛?

(2)以前都用甚麼材料?這個材料有甚麼特性

(3)為甚麼要新用蛋白質材料?這個材料有甚麼特性

(4)為甚麼要用角蛋白?

(5)根據不同的配比，我們應該預期什麼樣的結果?

(6)根據不同的角蛋白，我們應該預期什麼樣的結果?

(7)模擬跟實驗要怎麼連接?