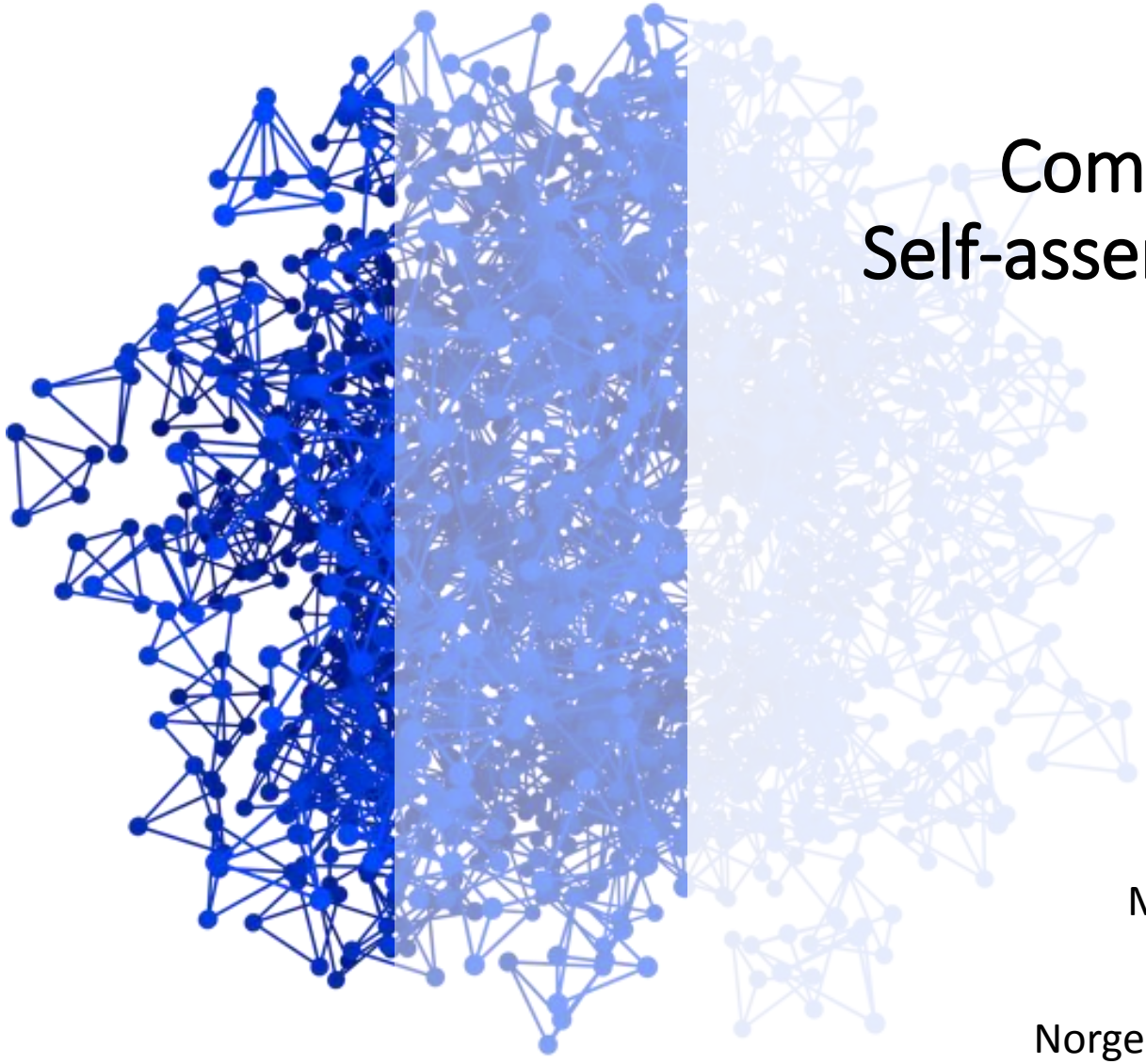

Computational Simulation for Self-assembled Nanogel with MOLSIM

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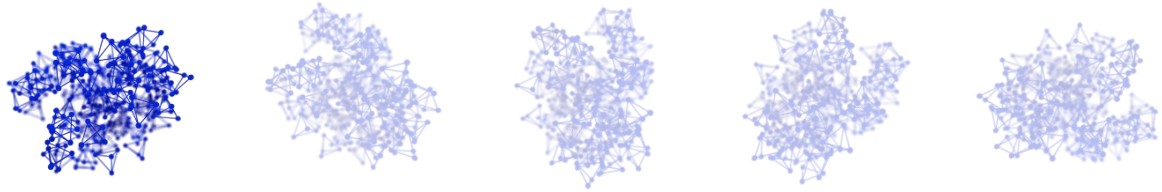
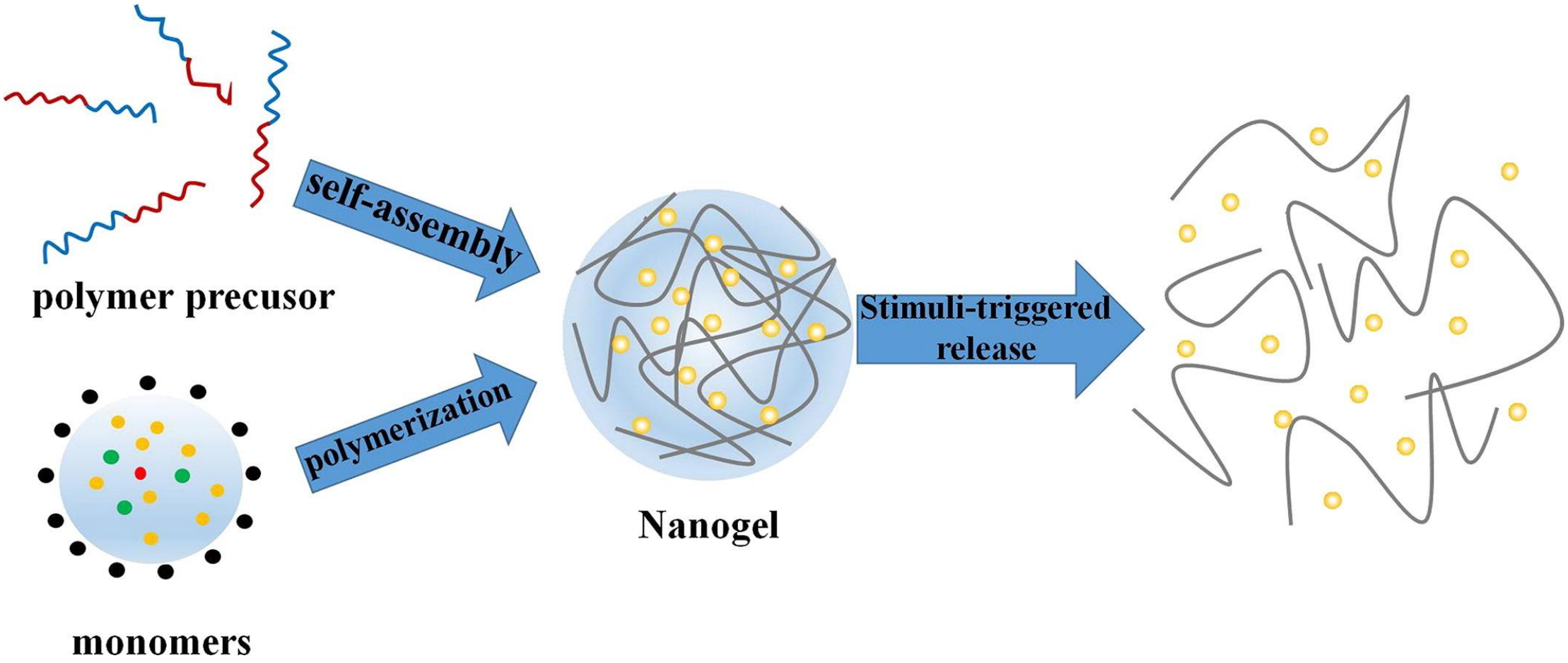
Department of Physics
Norges Teknisk-Naturvitenskapelige Universitet

NTNU
Norwegian University of Science and Technology

Introduction





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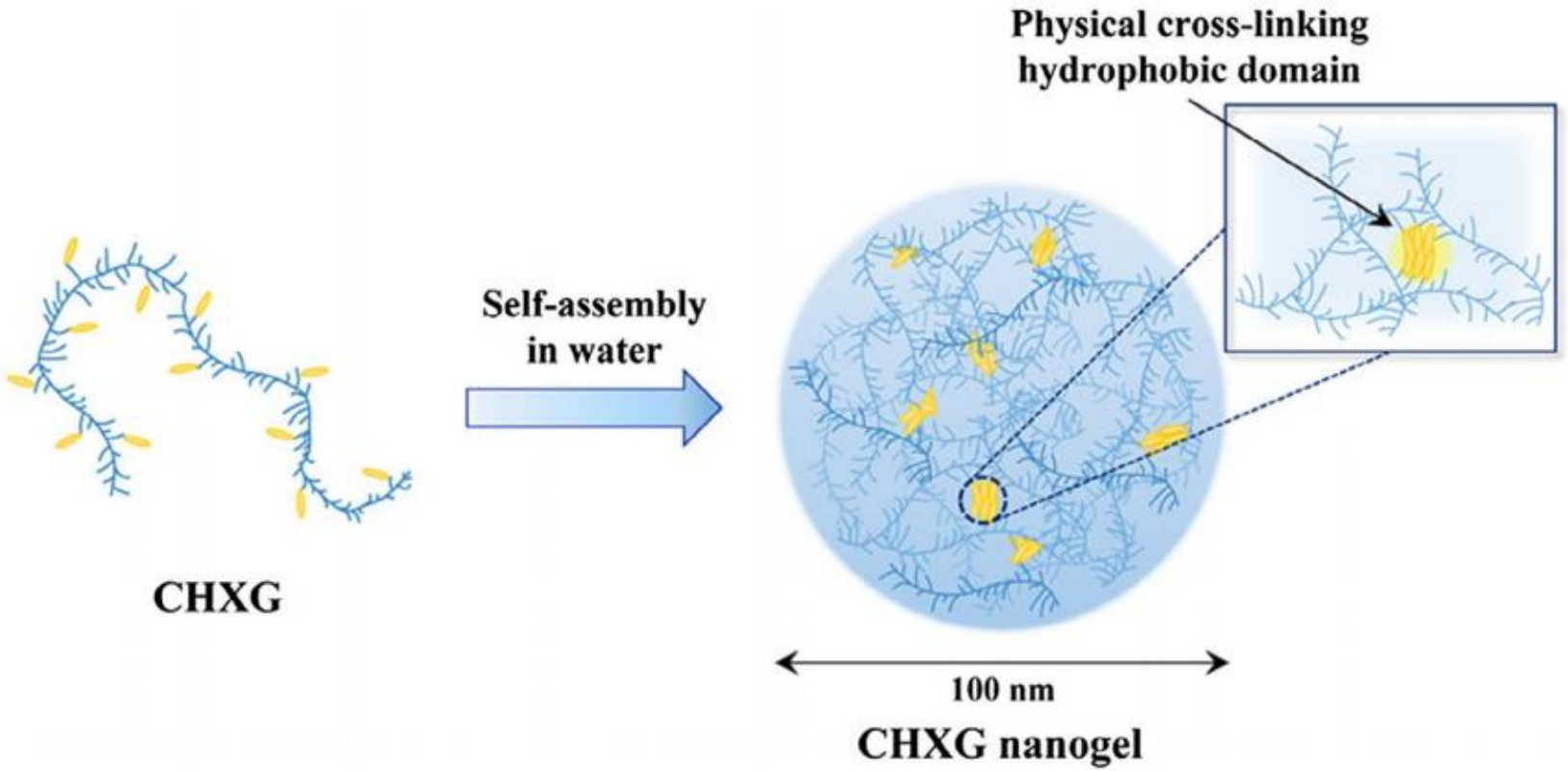
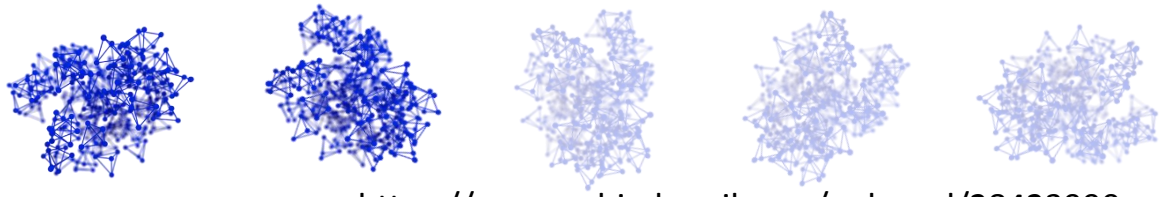
Introduction



https://www.ncbi.nlm.nih.gov/pubmed/28423990

System: Scheme



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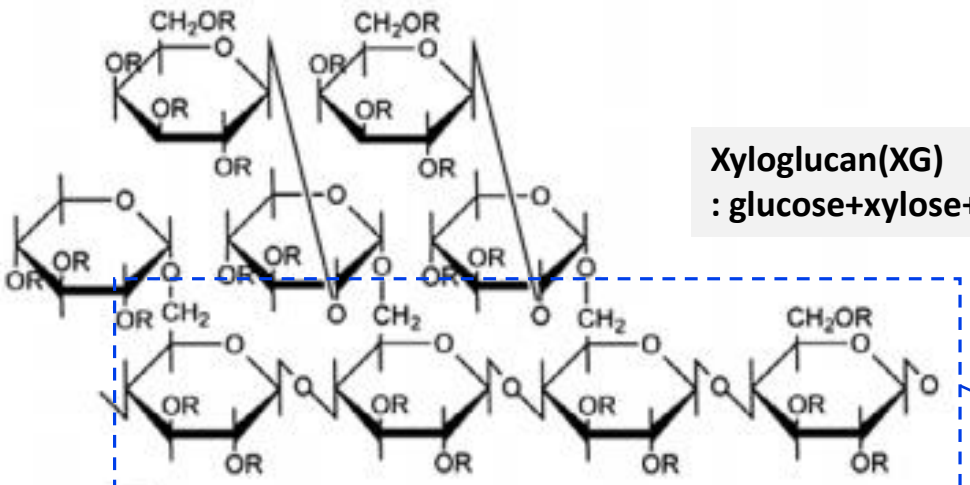
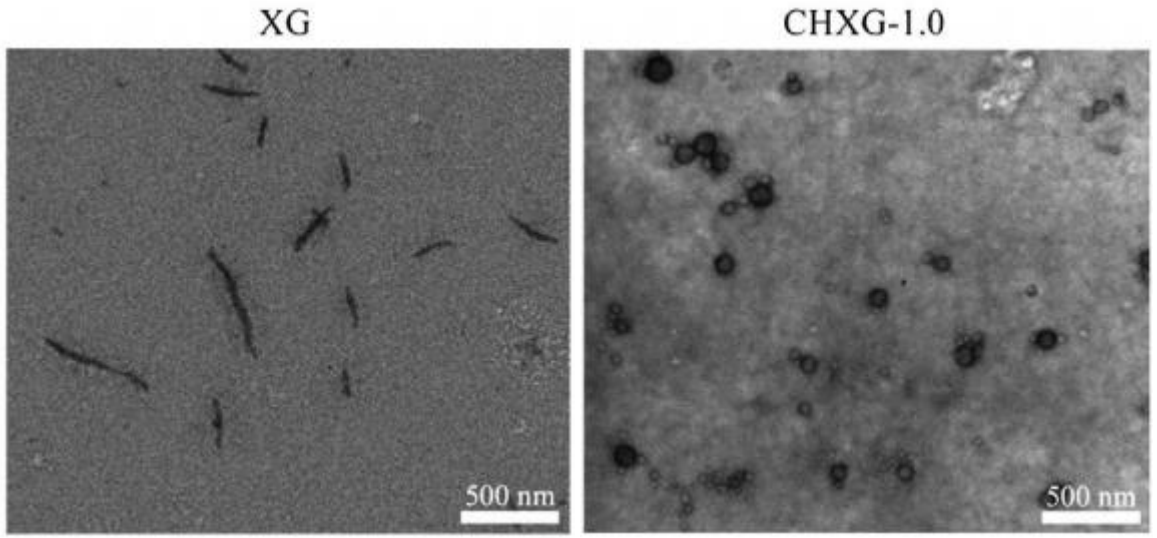


Xyloglucan(XG)
: glucose+xylose+galactose

Cholesterol group(CH)



Self-assembled Nanogel

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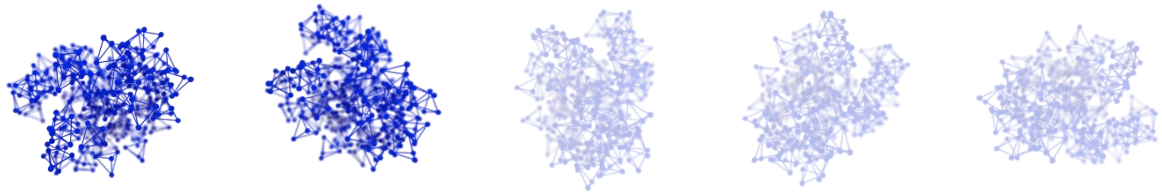
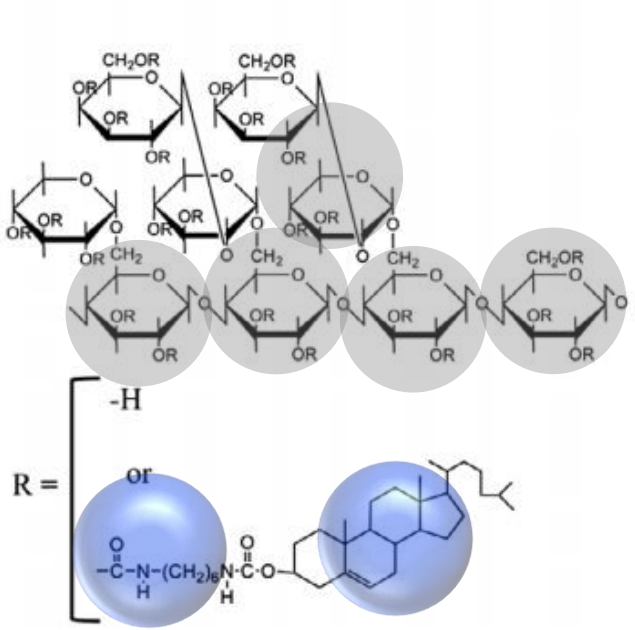
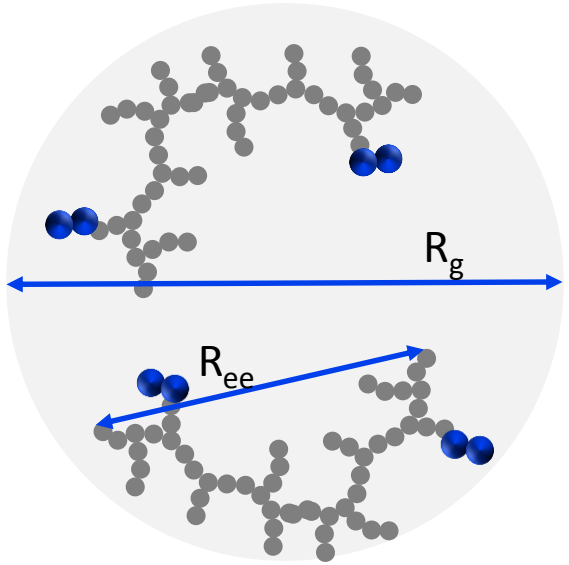
System: Simulation para.



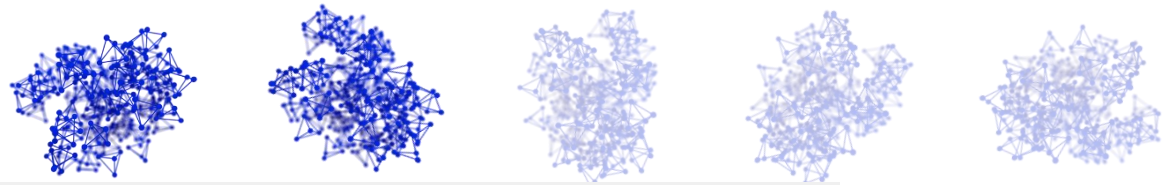




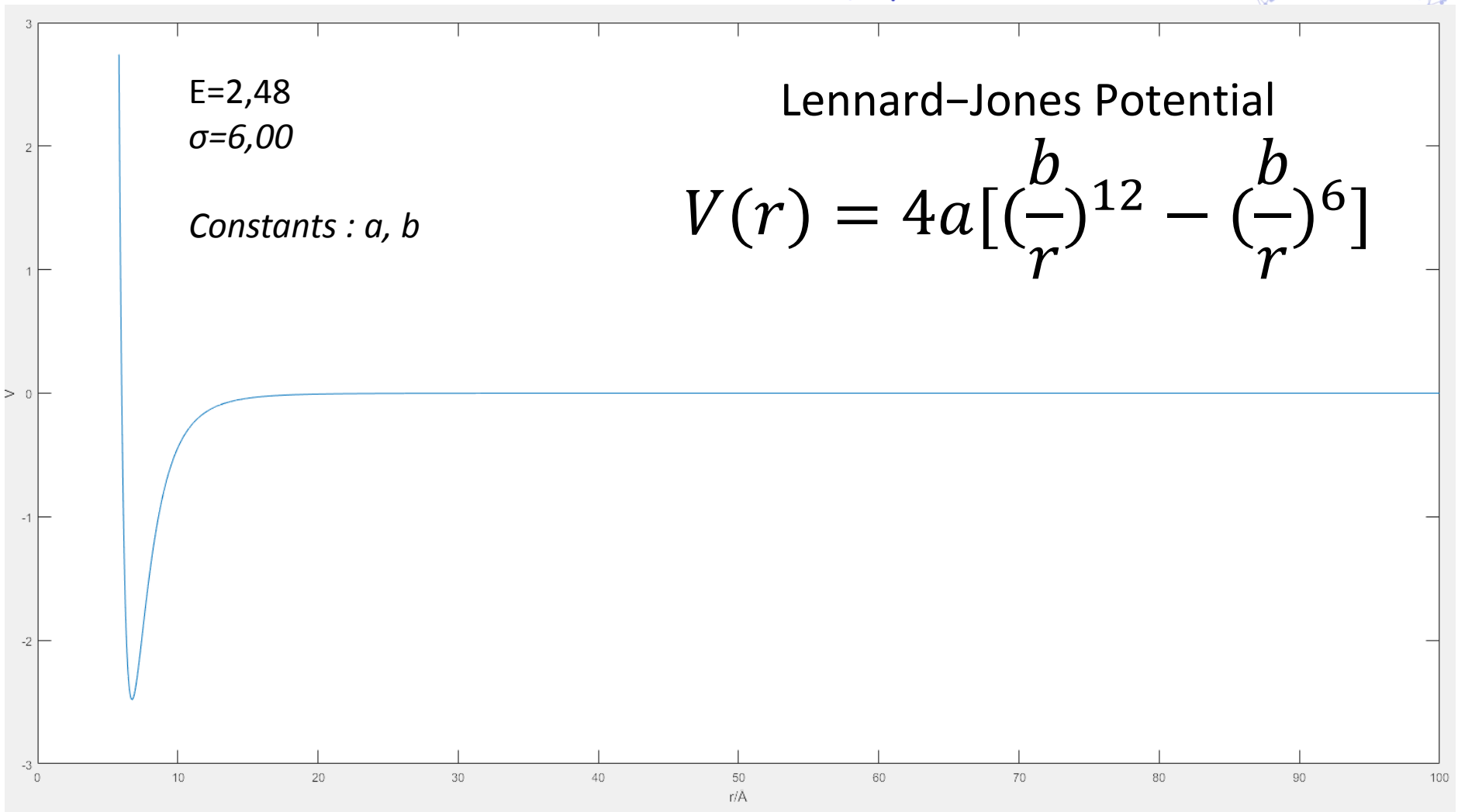
Simulation Mode
Monte Carlo
Canonical ensemble

	Parameters for Simulation							
Parameter	nct	npptct(1,1)	Npptct(1,2)	npt	nppt	natpt	massat	radat
Units	#	→	→	→	→	→	g/mol	Å
XG w/o CH (CHXG0)	2	50,0	**2,0**	2	560,0	1,1	10.0	2.0
XG w/ single CH (CHXG1)	2	50,0	**2,2**	2	560,160	1,1	10.0	2.0
XG w/ double CH (CHXG2)	2	50,0	**2,4**	2	560,320	1,1	10.0	2.0

System: L-J Potential

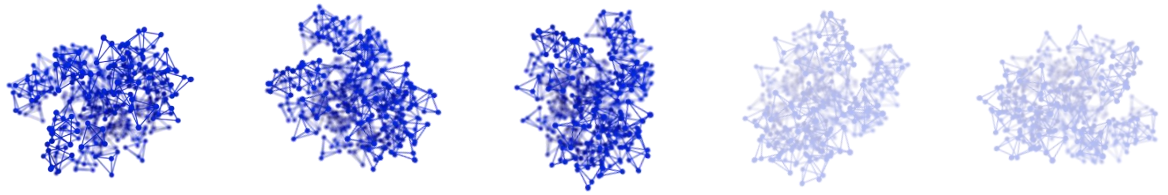


V(r)
[kJ/mol]



r [Å]

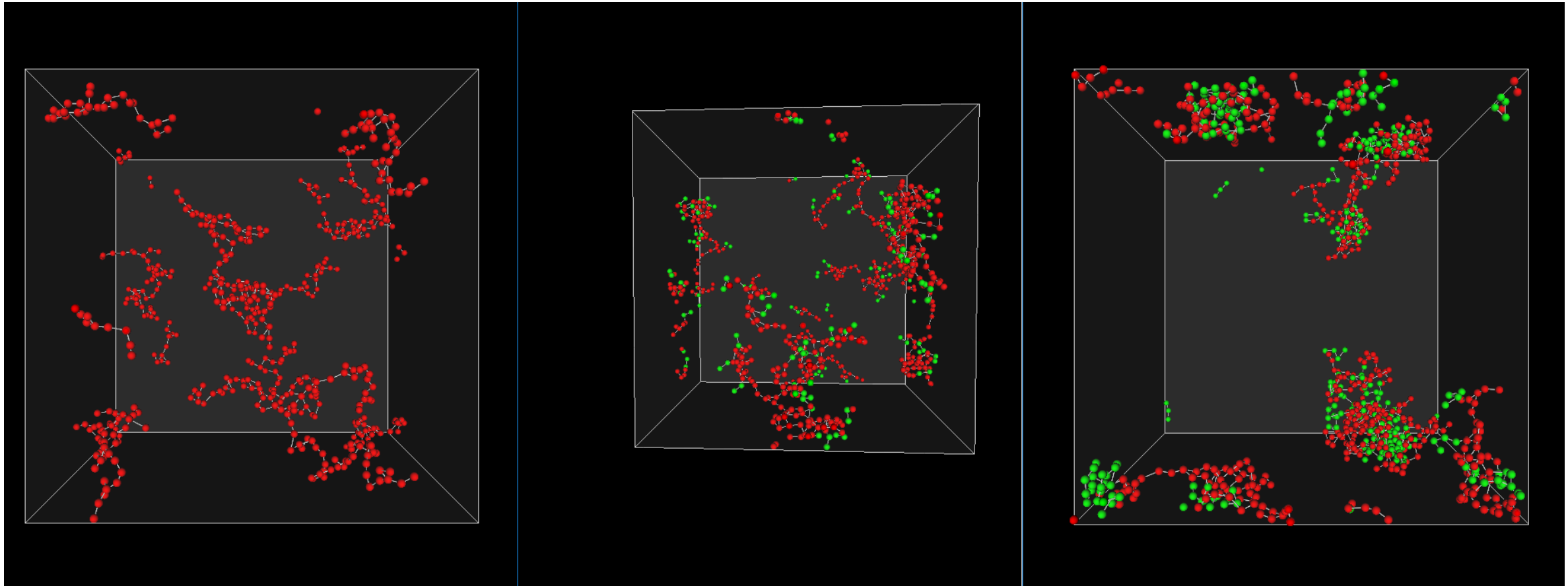
Results: 3D Images



XG w/o CH (CHXG0)

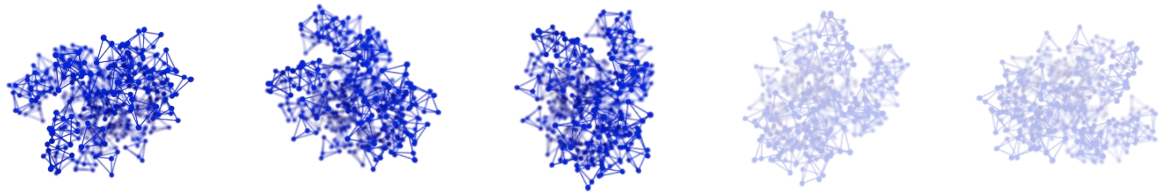
XG w/ single CH (CHXG1)

XG w/ double CH (CHXG2)



N = 10 000

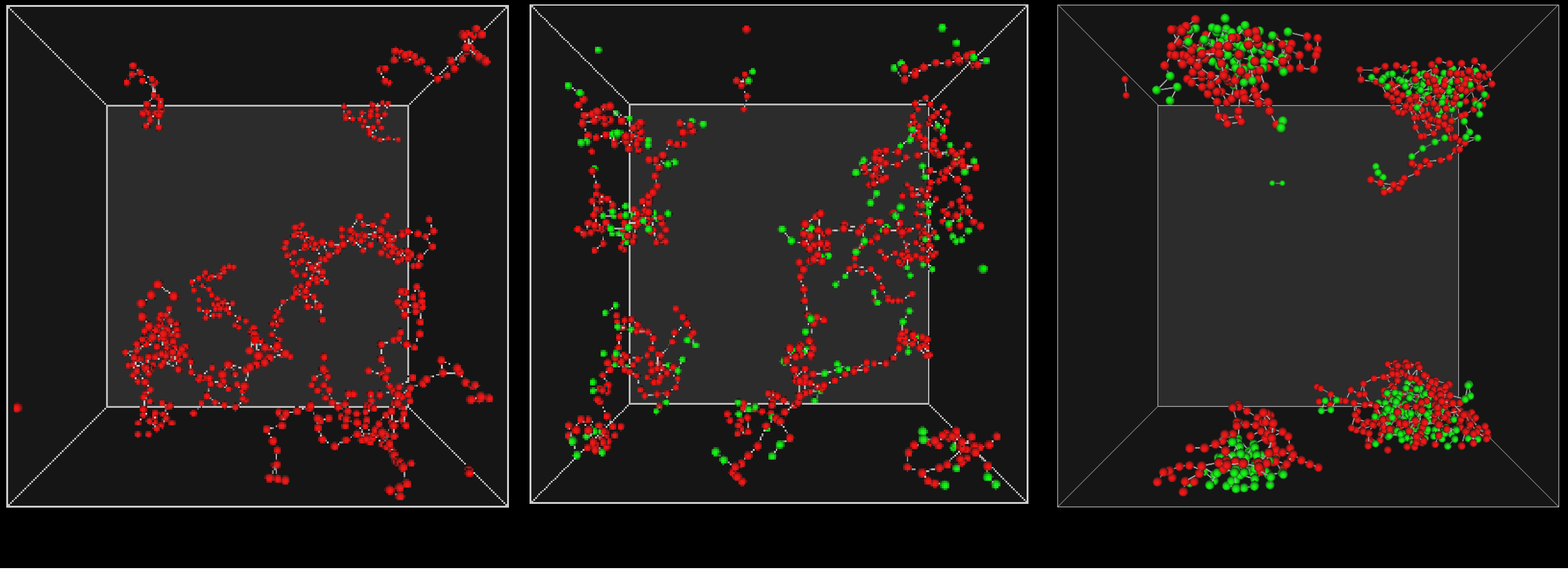
Results: 3D Images



XG w/o CH (CHXG0)

XG w/ single CH (CHXG1)

XG w/ double CH (CHXG2)



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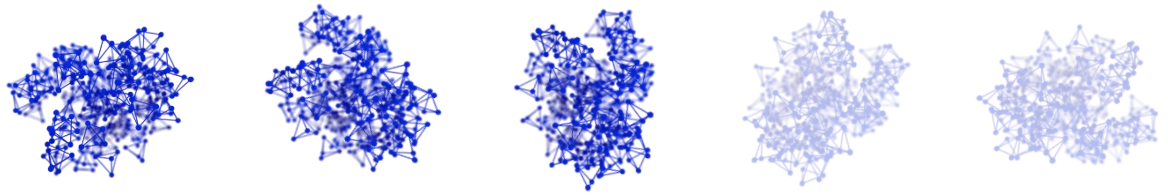
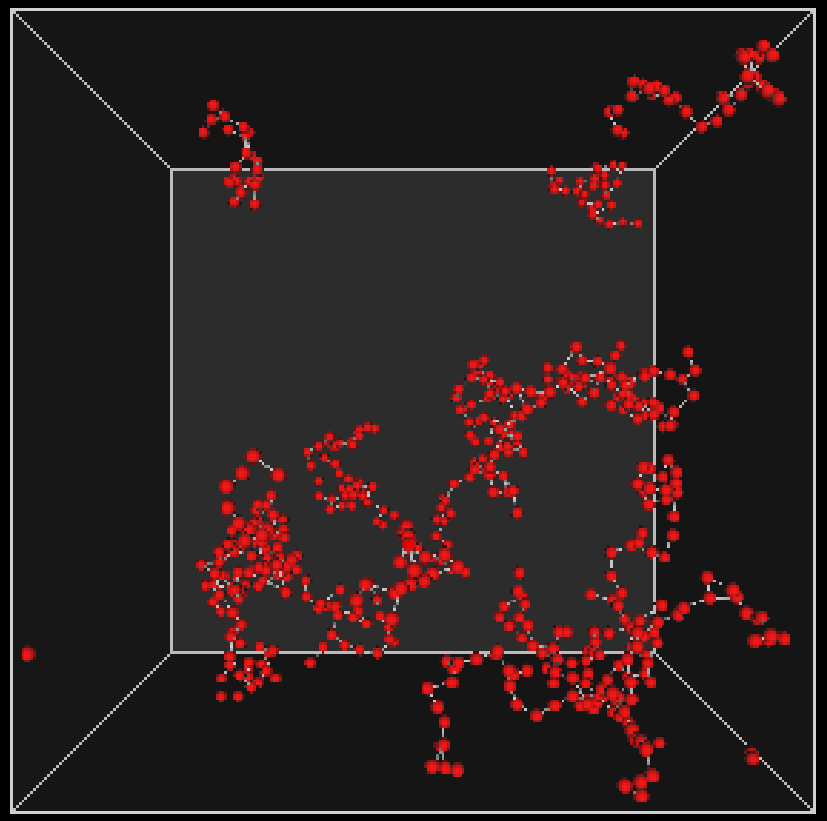
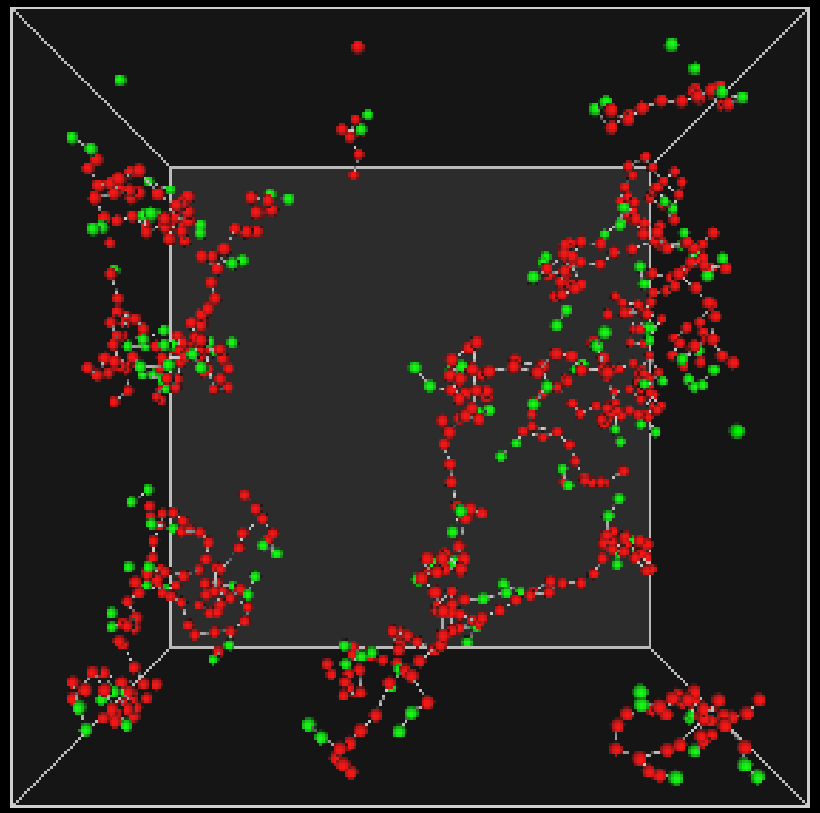


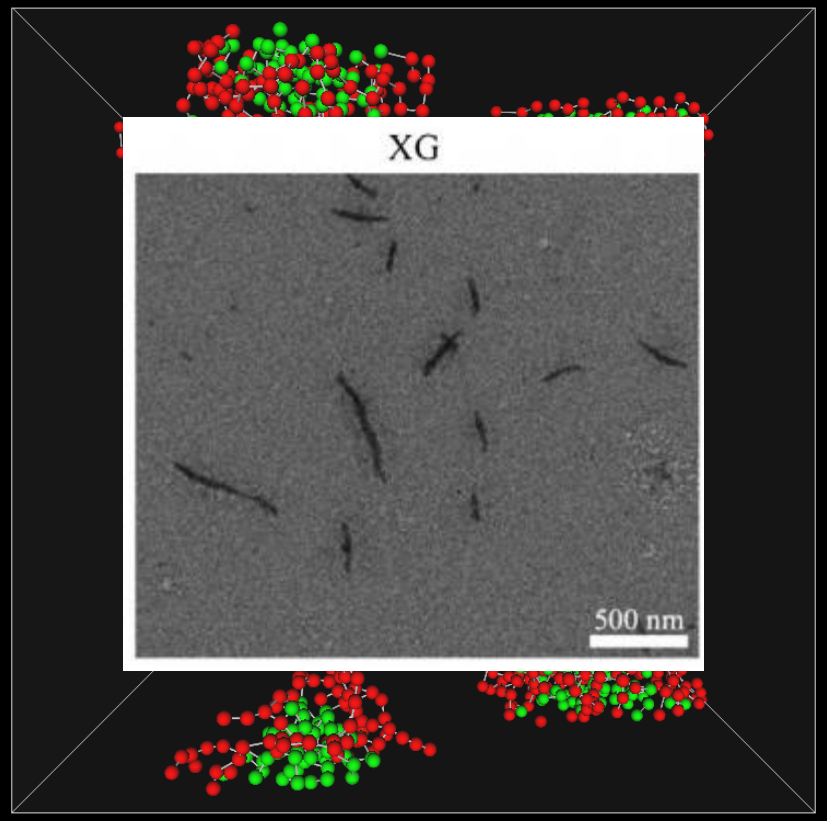
XG w/o CH (CHXG0)

XG w/ single CH (CHXG1)

XG w/ double CH (CHXG2)







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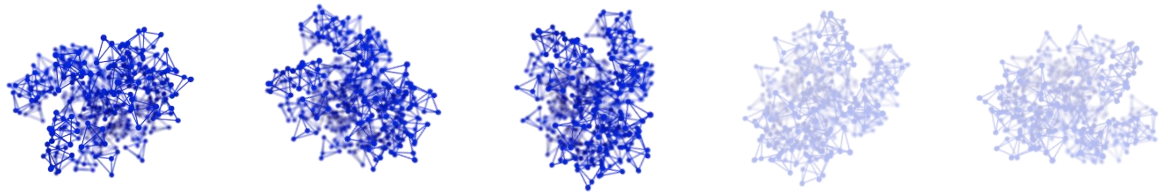
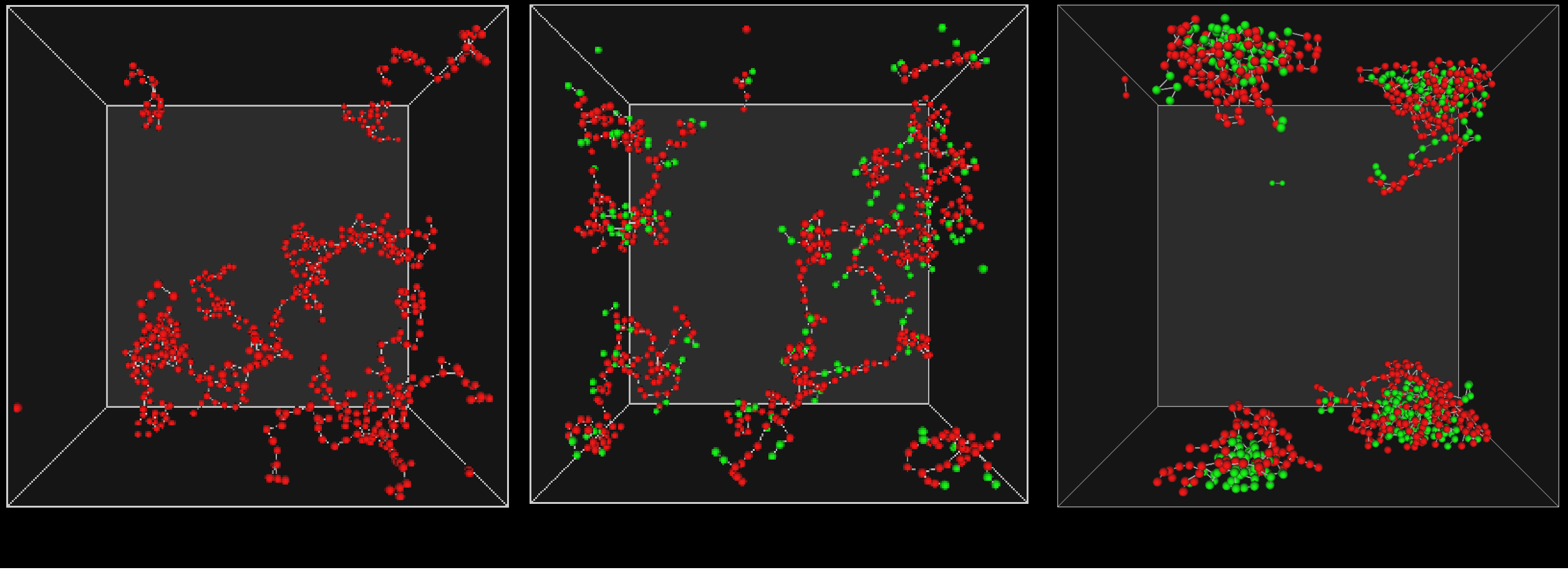
Results: 3D Images



XG w/o CH (CHXG0)

XG w/ single CH (CHXG1)

XG w/ double CH (CHXG2)



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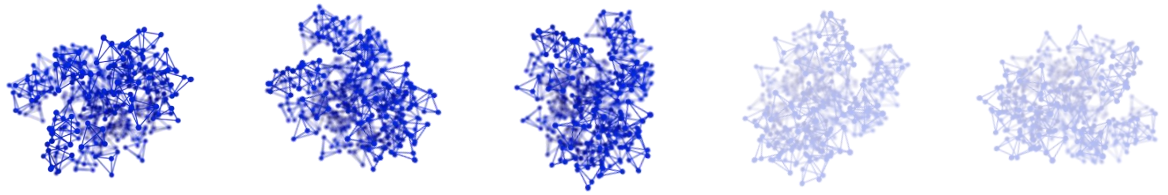
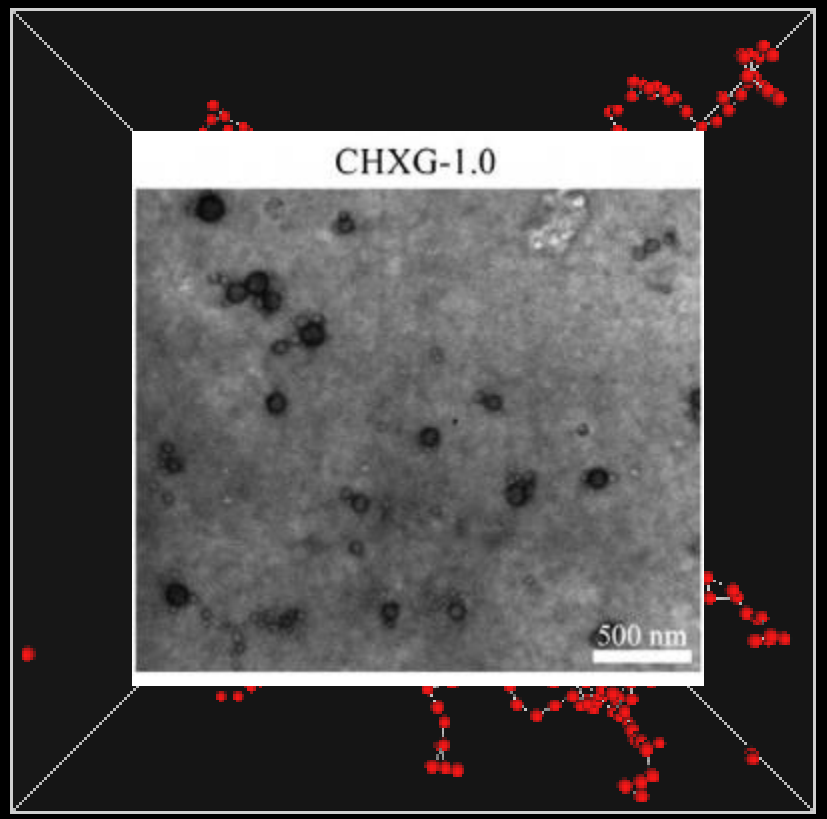
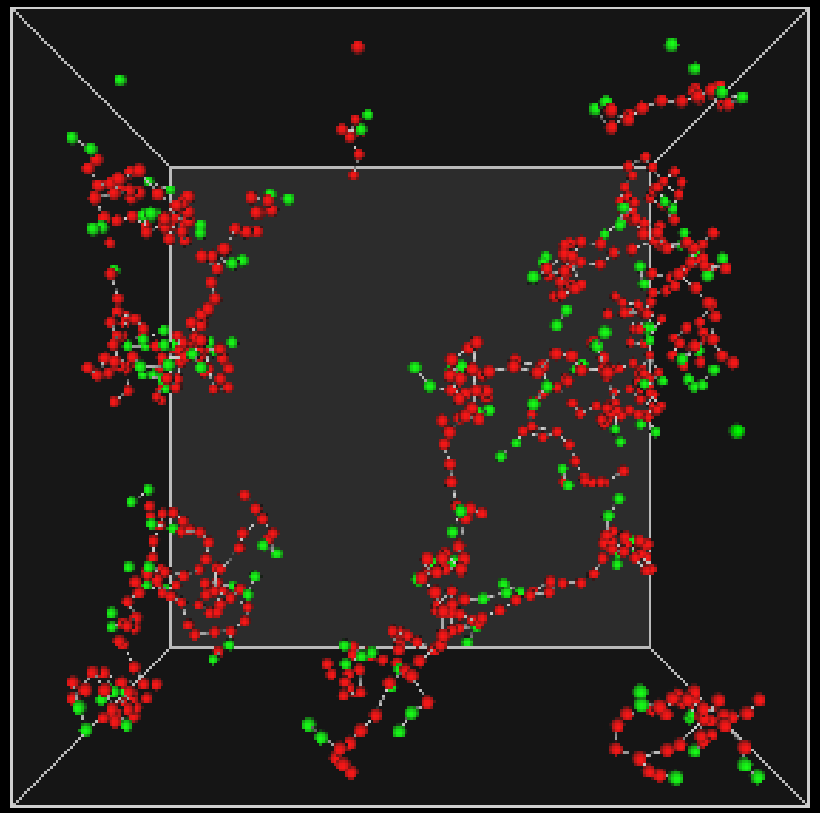


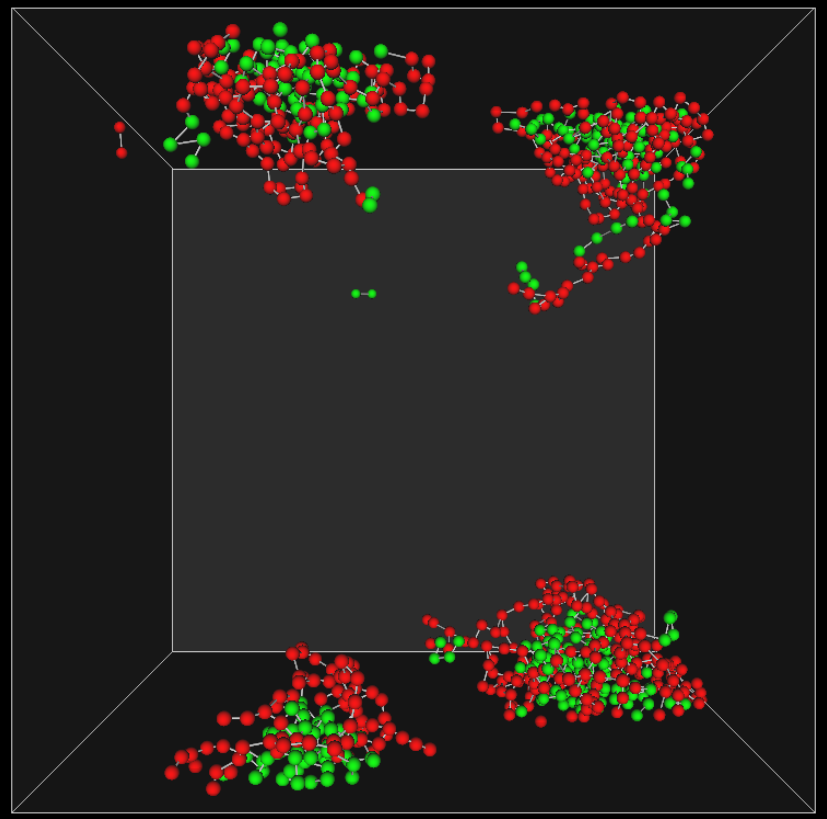
XG w/o CH (CHXG0)

XG w/ single CH (CHXG1)

XG w/ double CH (CHXG2)

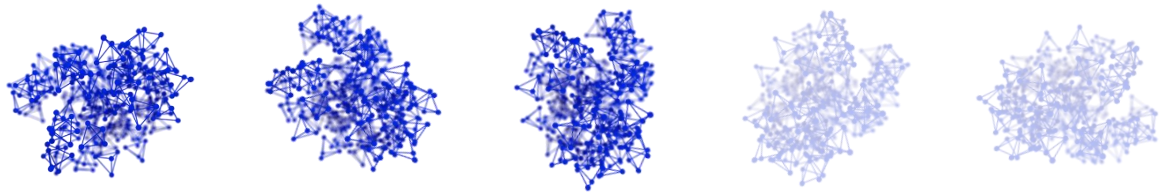


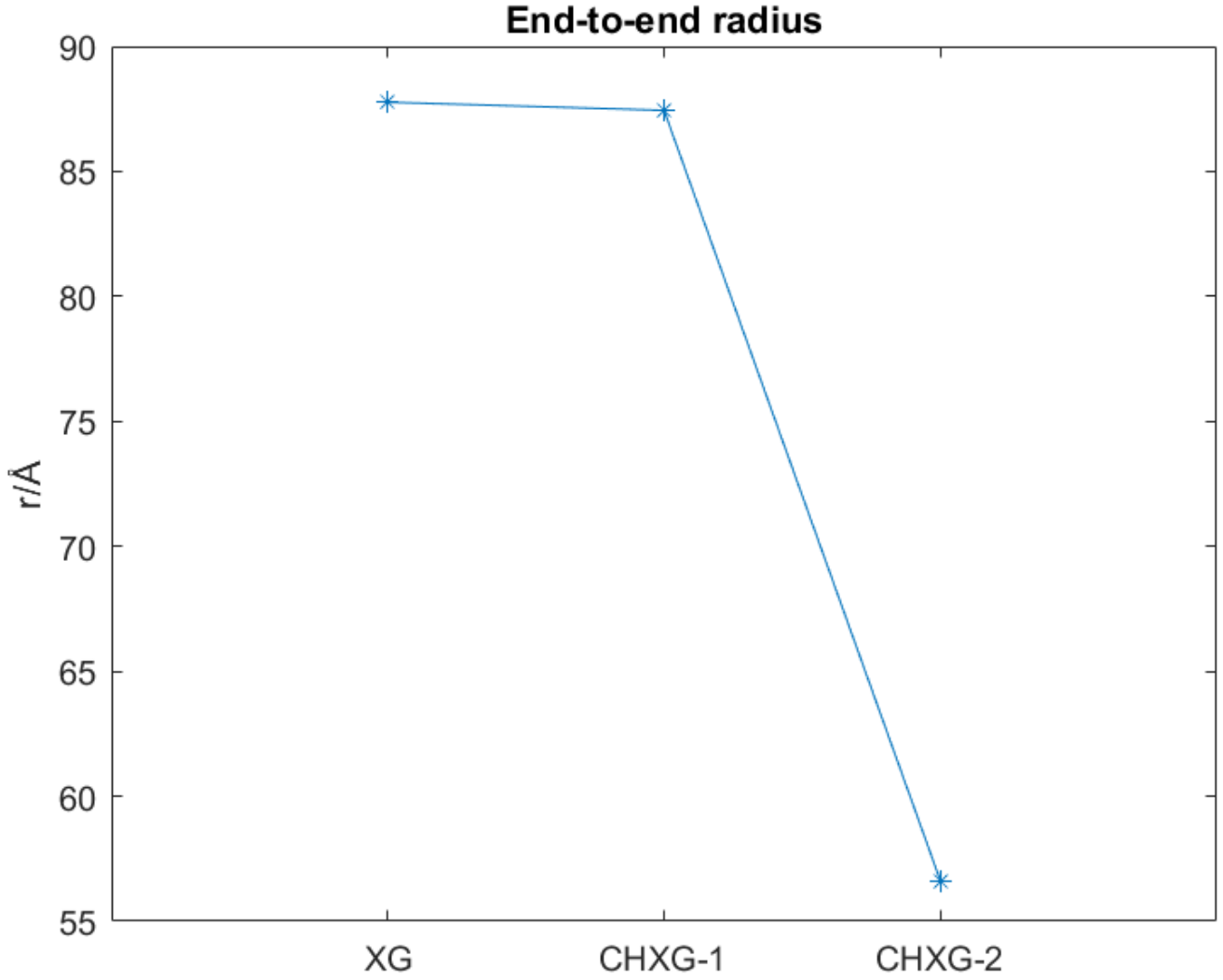


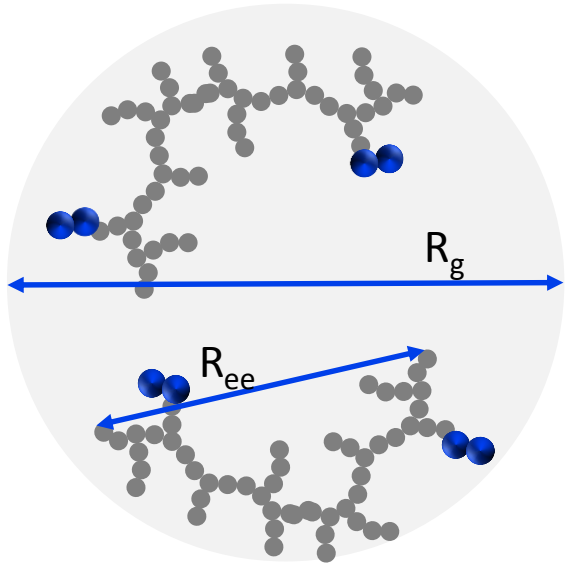


N = 400 000

Results: Ree







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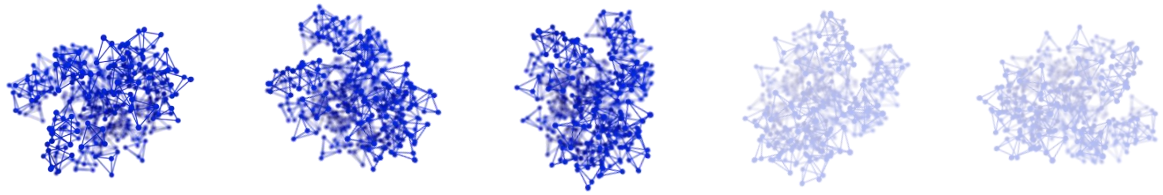

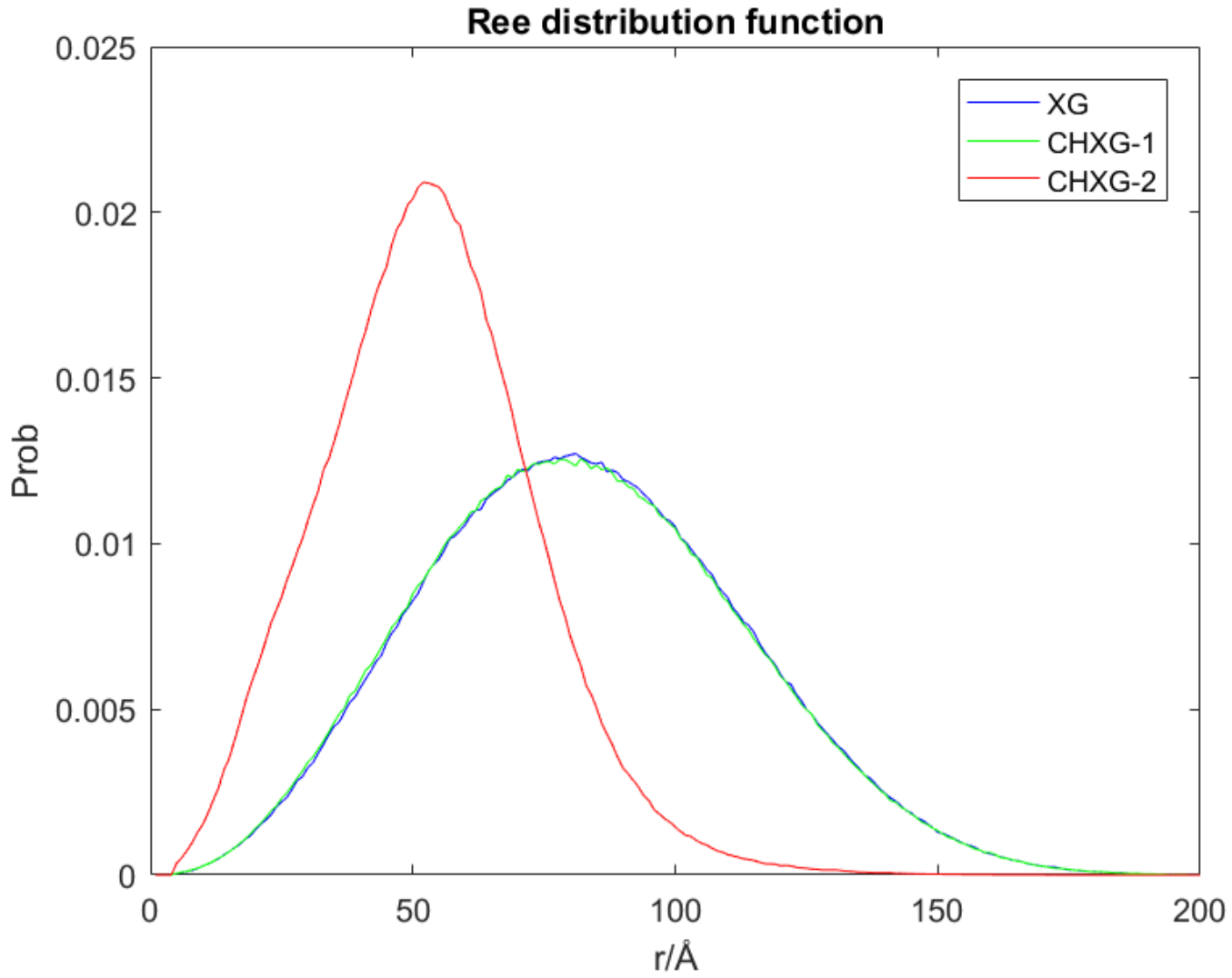

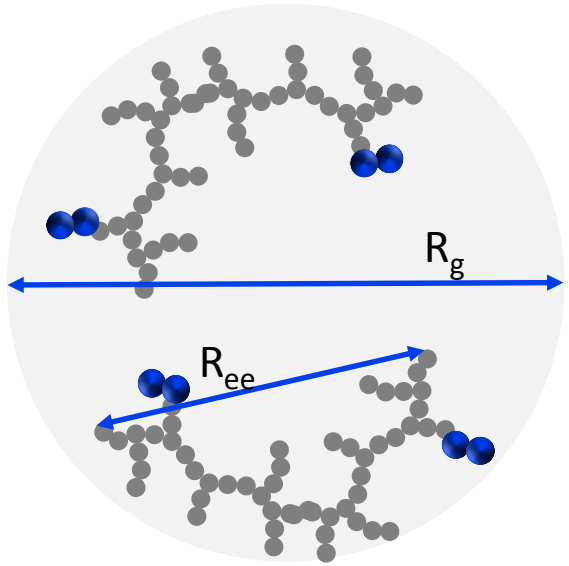

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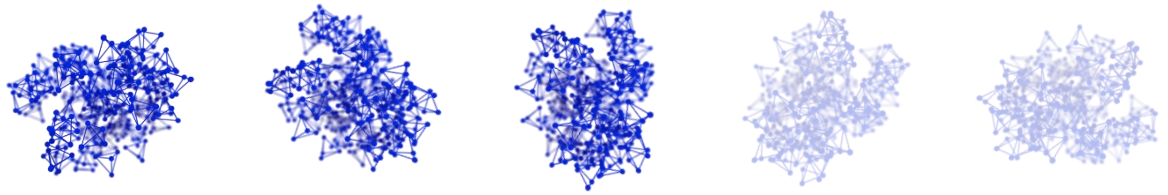
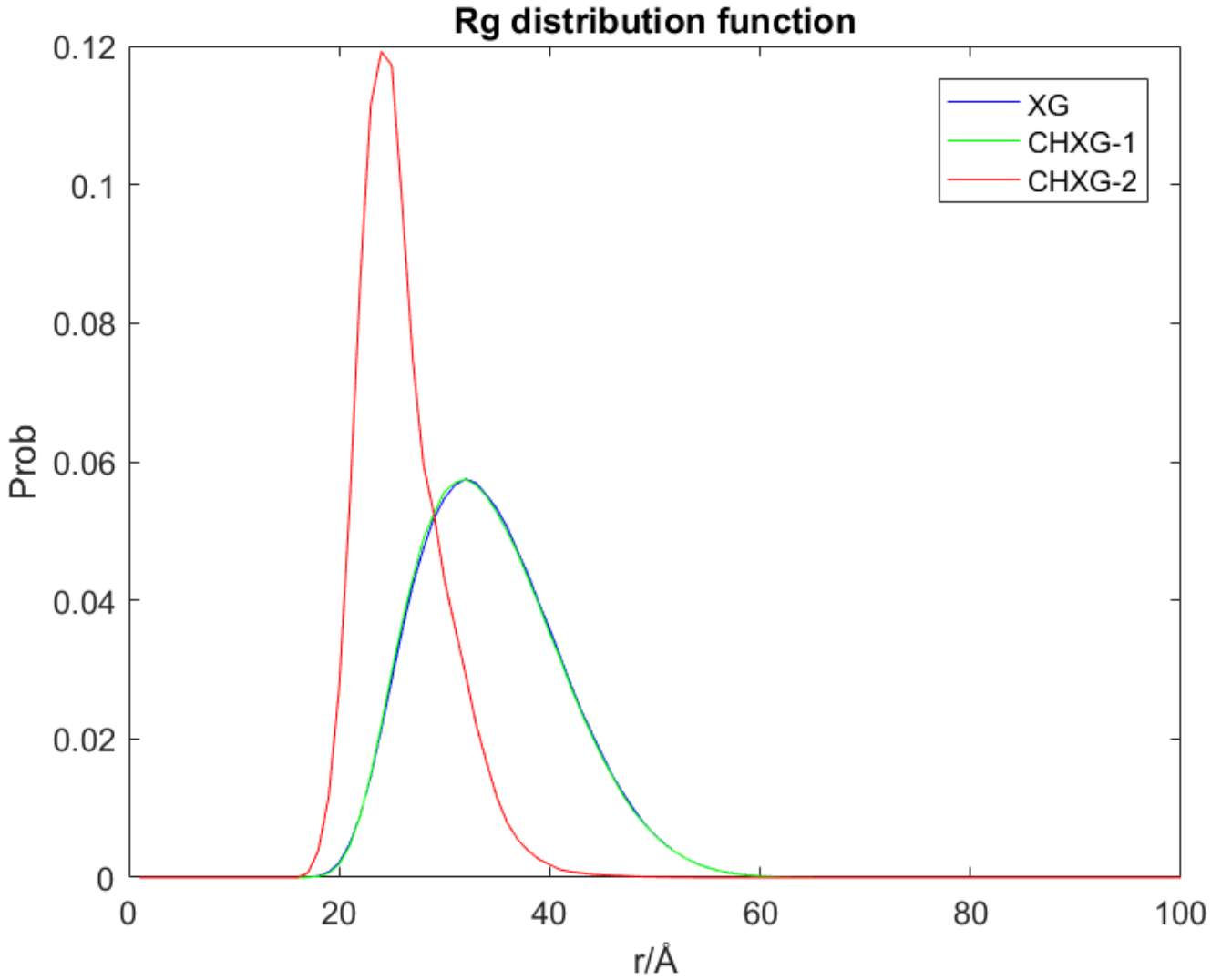
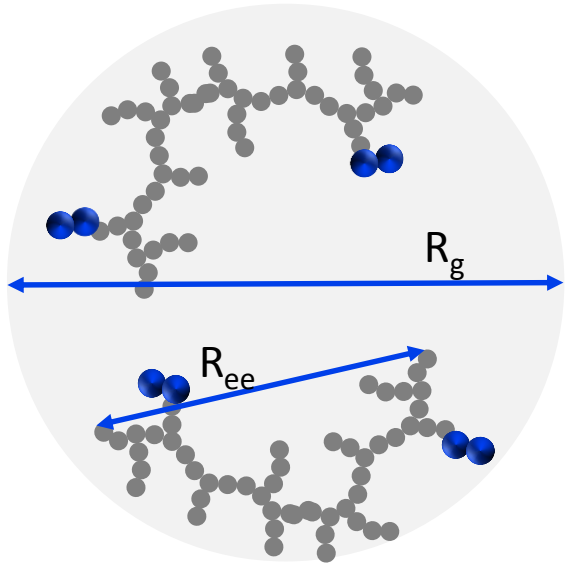
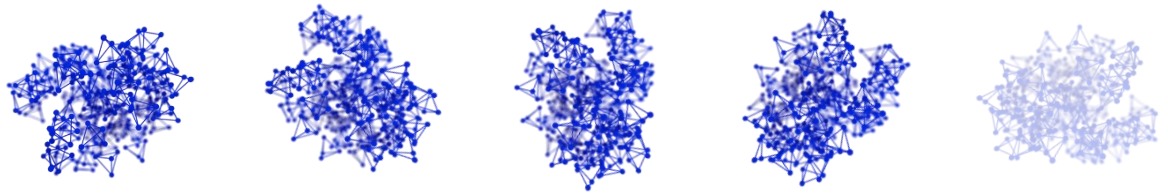
Results: Radius of gyration







Conclusion & Future Work



- Increasing Cholesterol group - self assembly ↑

→ Relationship between **# of Cholesterol – Self assembly(Rg)**

: Questions about limitation of increasing CH group

- How do we **improve self-assembly**?

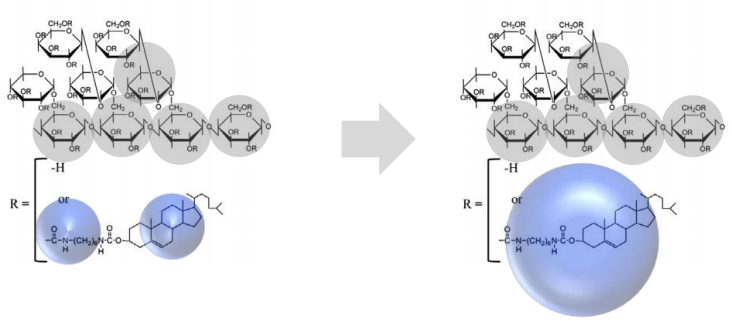
→ Increasing # of CH group

→ Structure of Cholesterol/Xyloglucan

: # or side chain, Structure(Un/Saturated), Persistent length

- How do we **improve simulation method?**

→ Changing assumption for Cholesterol structure



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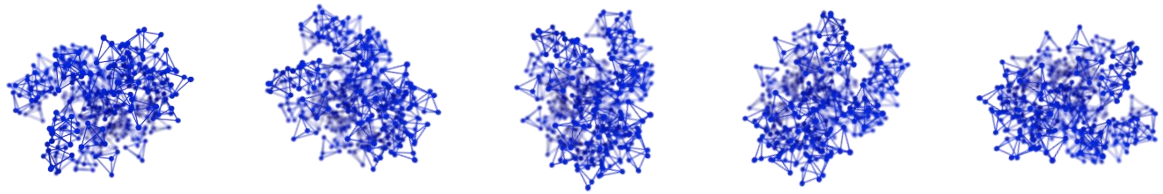
References



- Background image

http://molsim.lifesciences.autodesk.com

- Introduction

- New progress and prospects: The application of nanogel in drug delivery, Hui Zhang, Materials Science and Engineering :C, 2015 Nov

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- Self-assembled nanogel of cholesterol-bearing xyloglucan as a drug delivery nano carrier, Sawada SI, J Biomater Sci Polym, 2017 April

https://www.ncbi.nlm.nih.gov/pubmed/28423990

- Systems

- Self-assembled nanogel of cholesterol-bearing xyloglucan as a drug delivery nano carrier, Sawada SI, J Biomater Sci Polym

https://www.ncbi.nlm.nih.gov/pubmed/28423990