Influence of chain stiffness and sequence on knottedness in polymer globules

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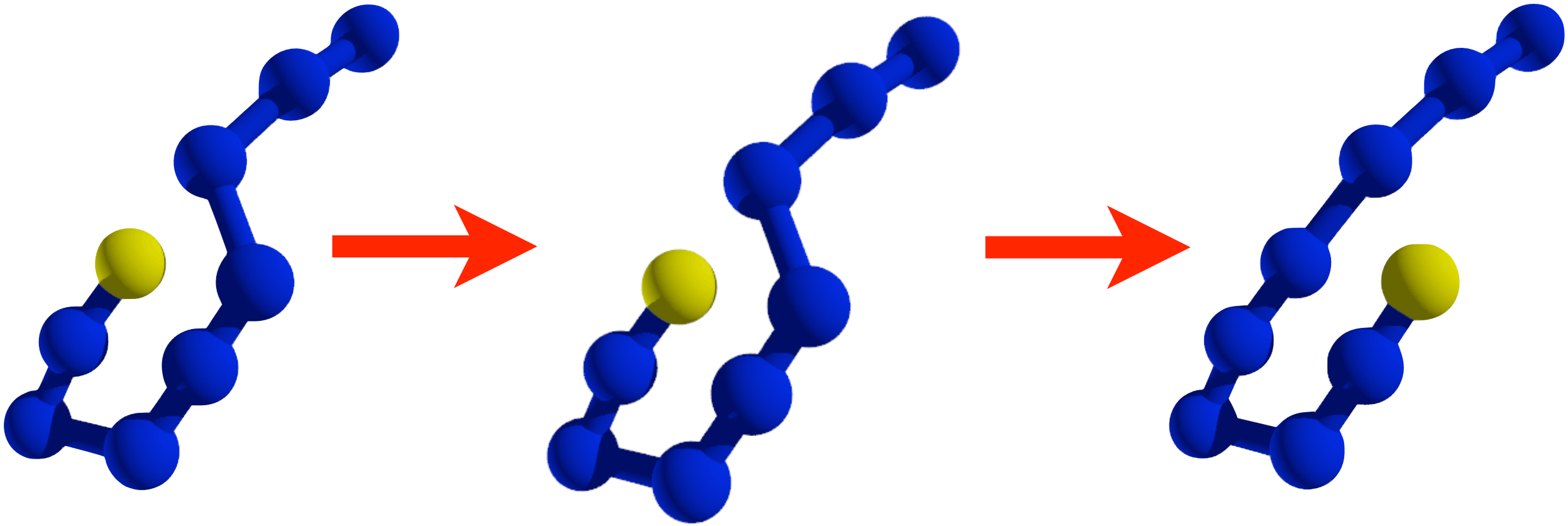
Backbite move



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for lattice models: M.L. Mansfield, J. Chem. Phys., **77**, 1554 (1982)

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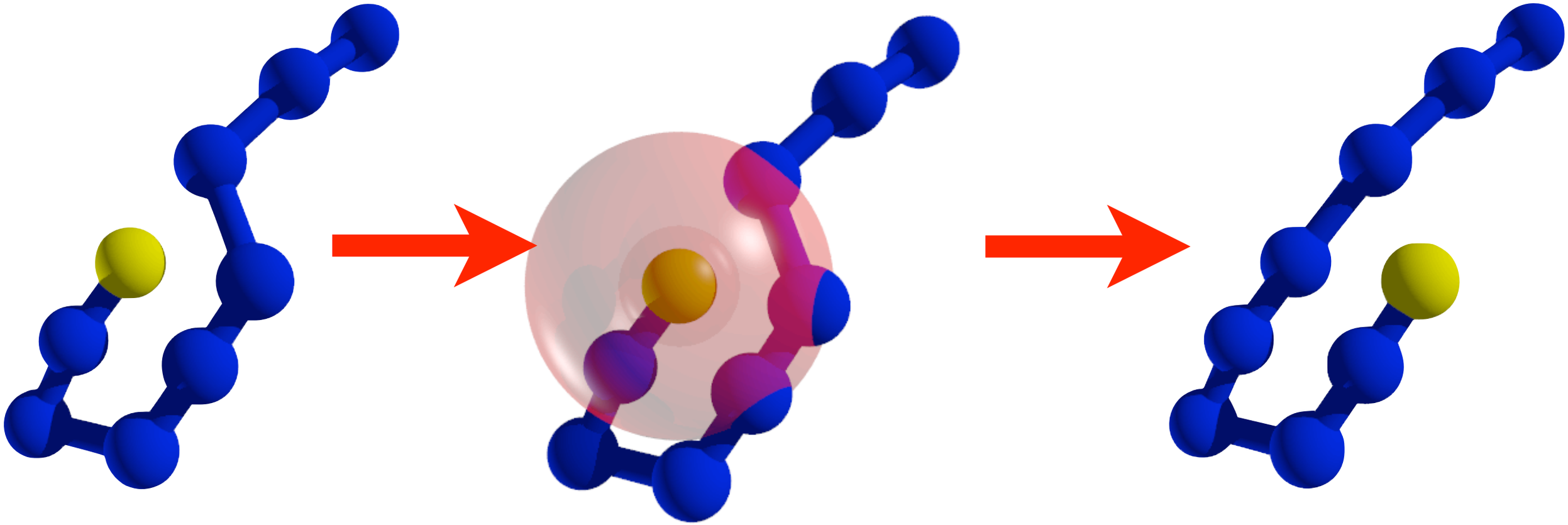

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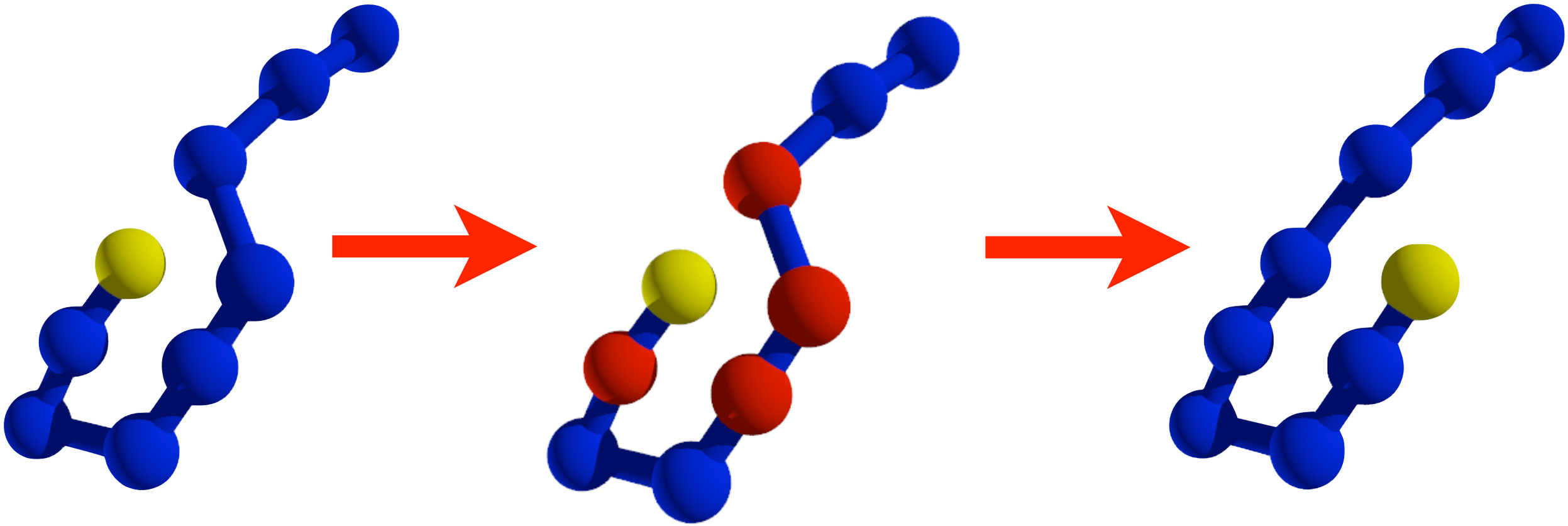

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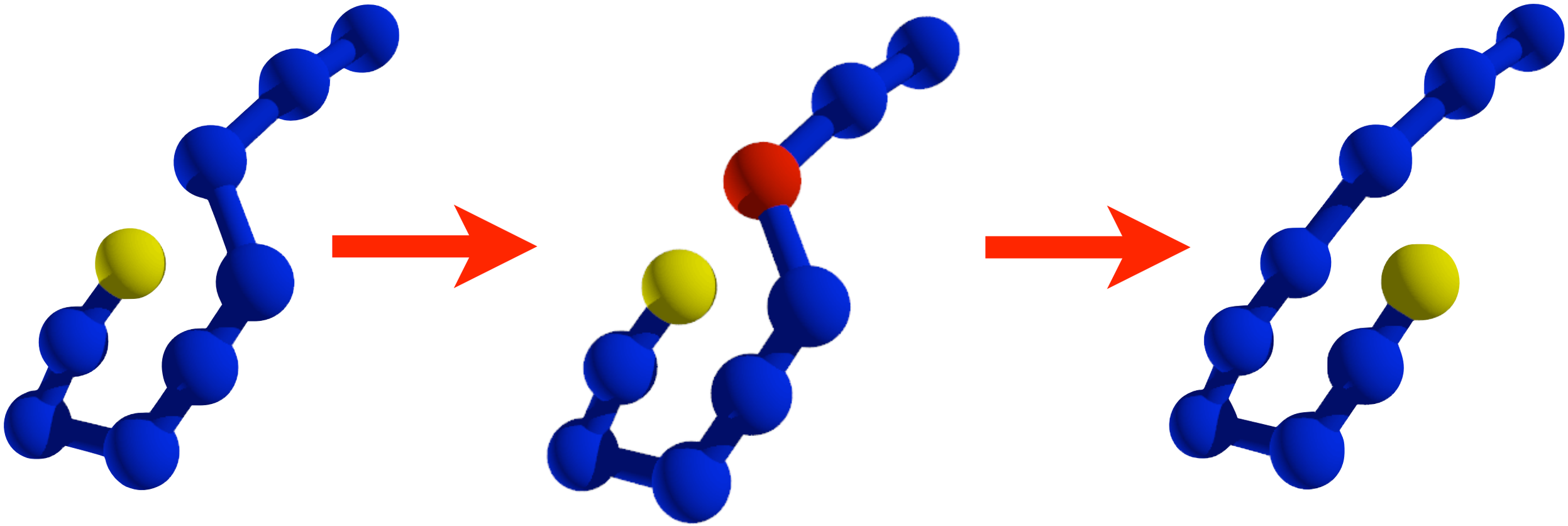

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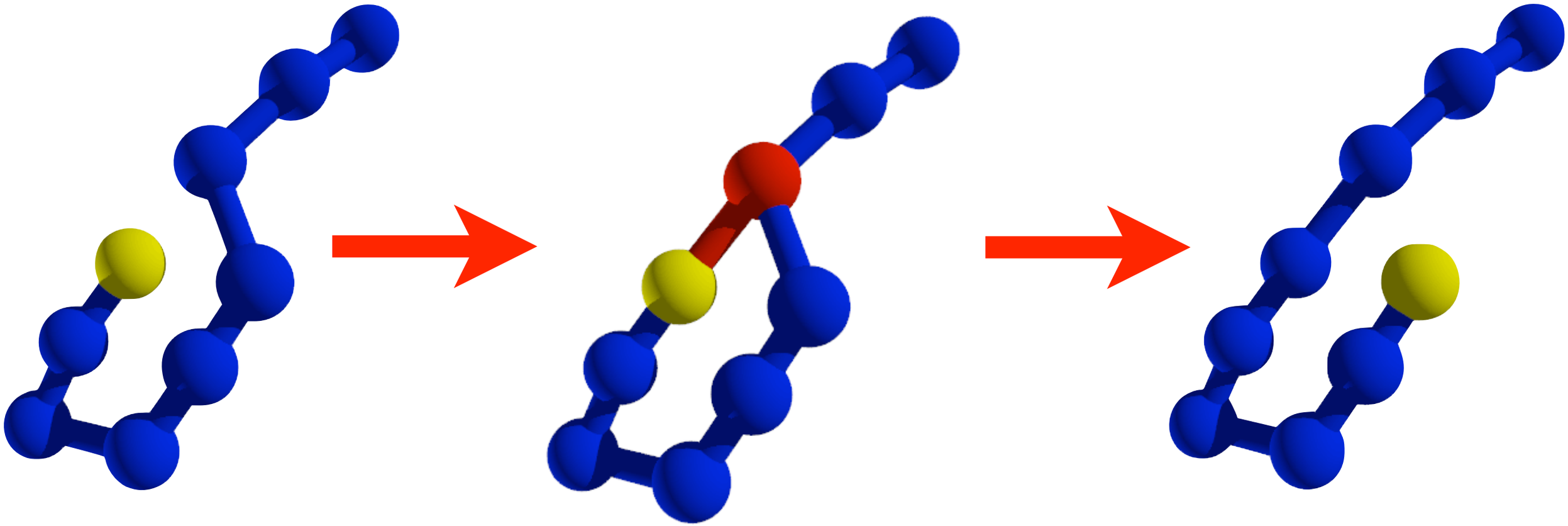

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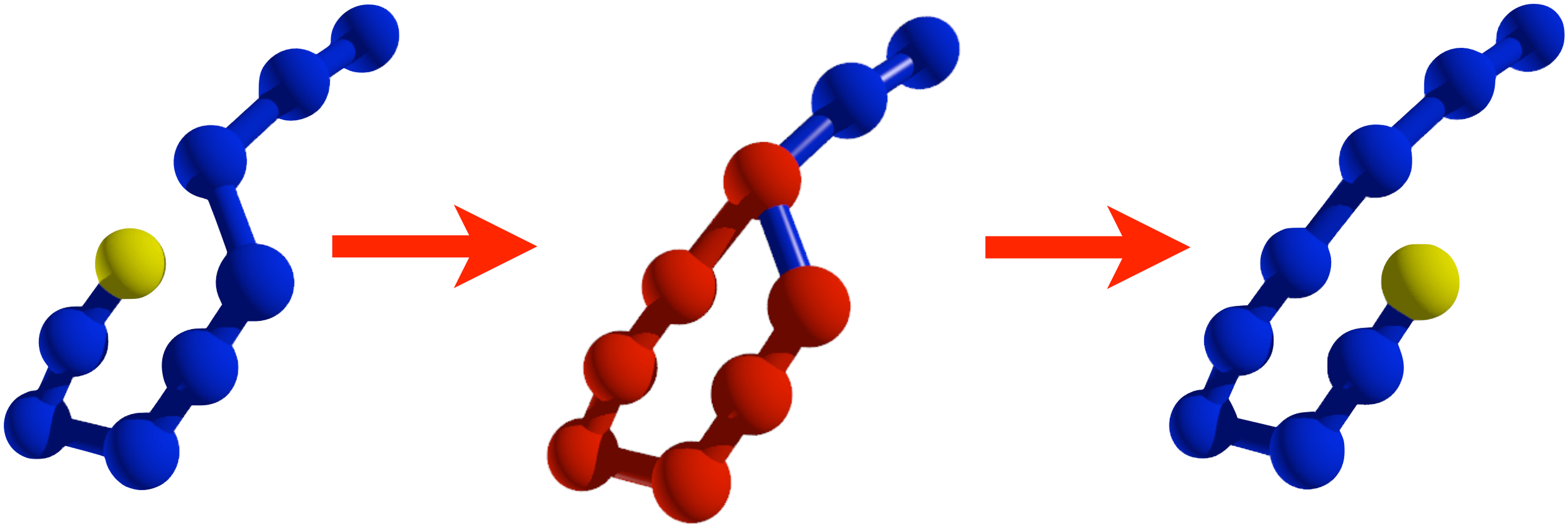

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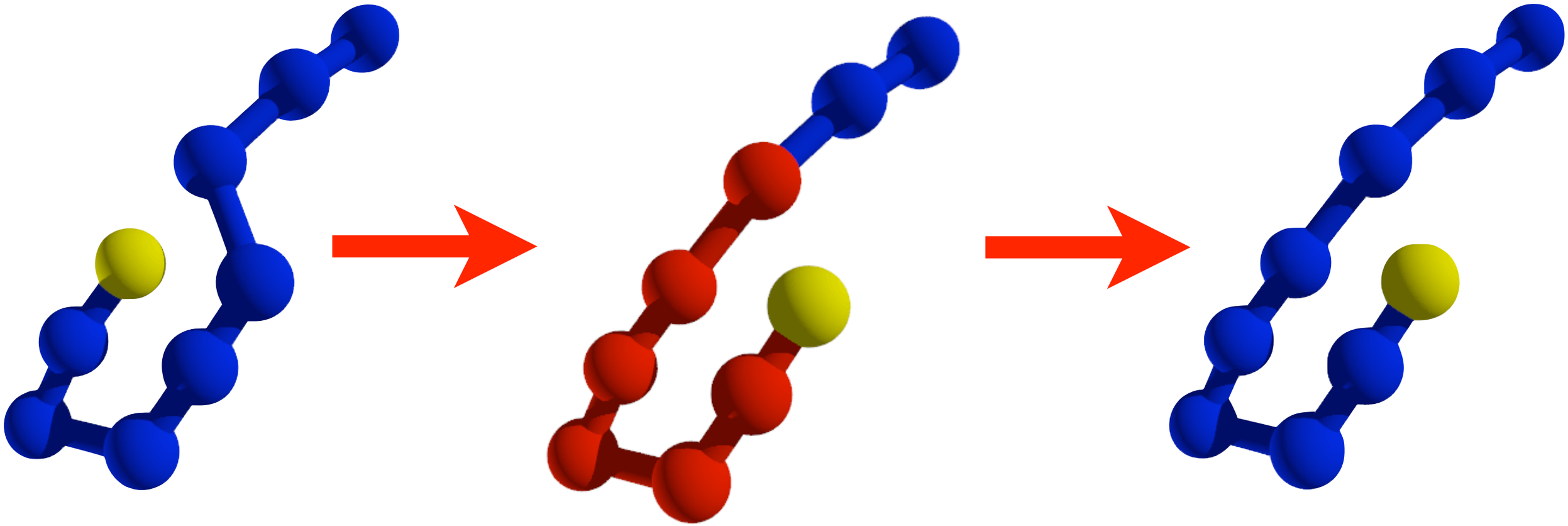

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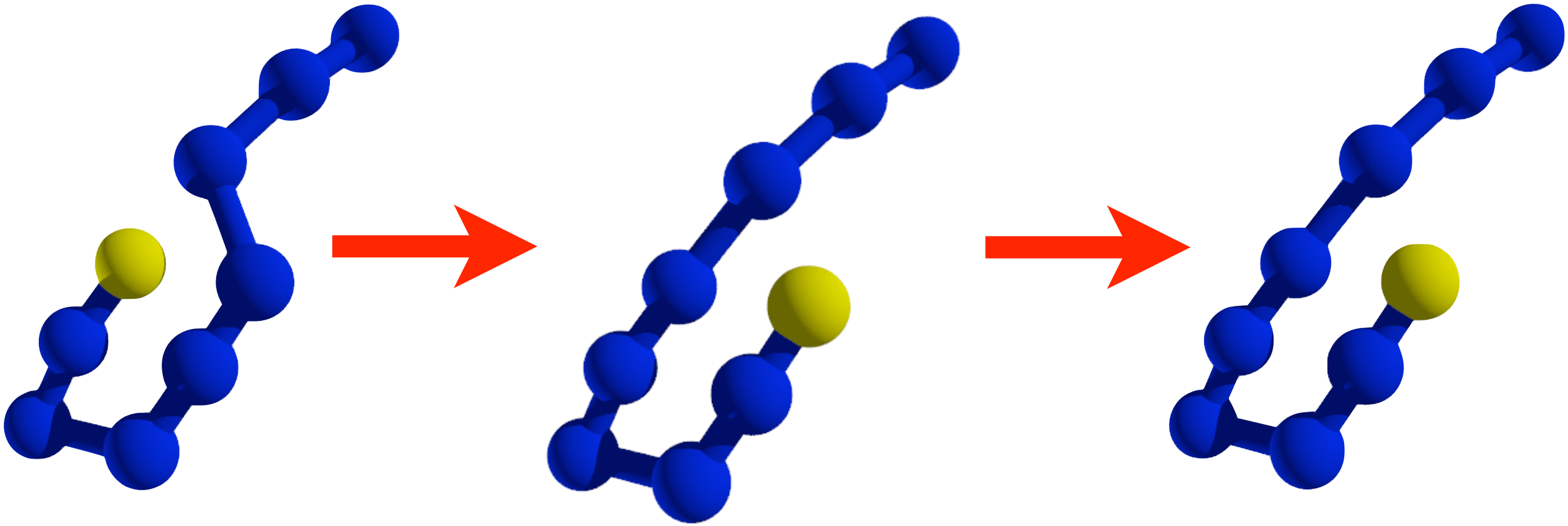

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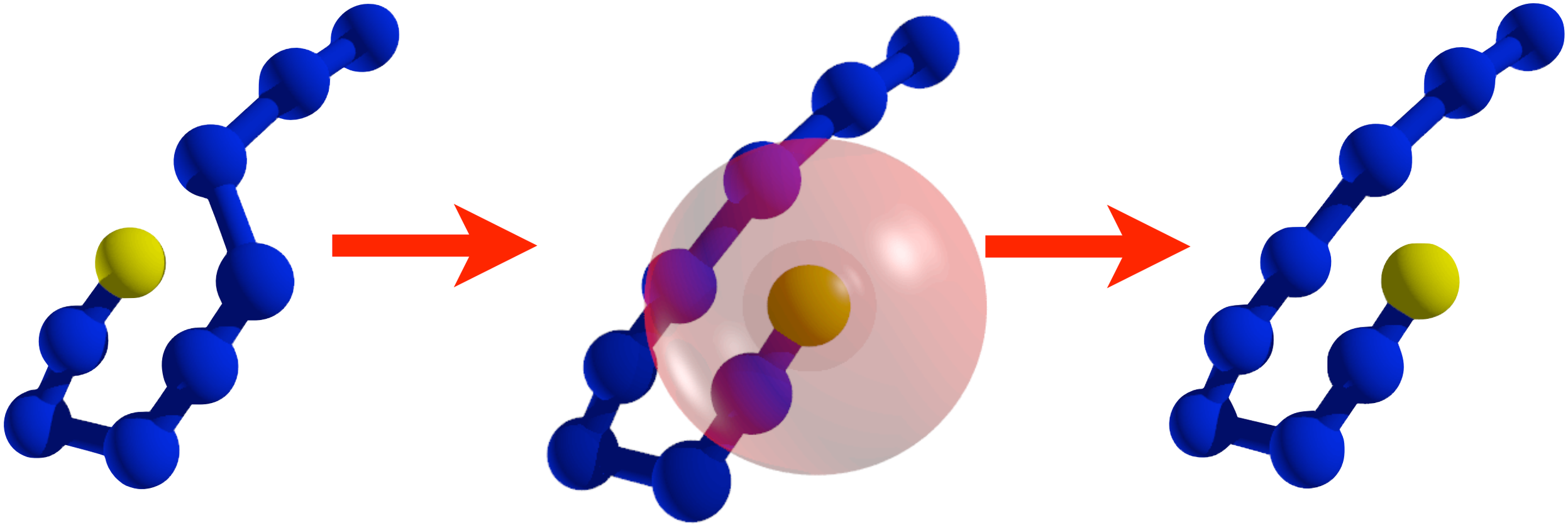

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for lattice models: M.L. Mansfield, J. Chem. Phys., **77**, 1554 (1982)

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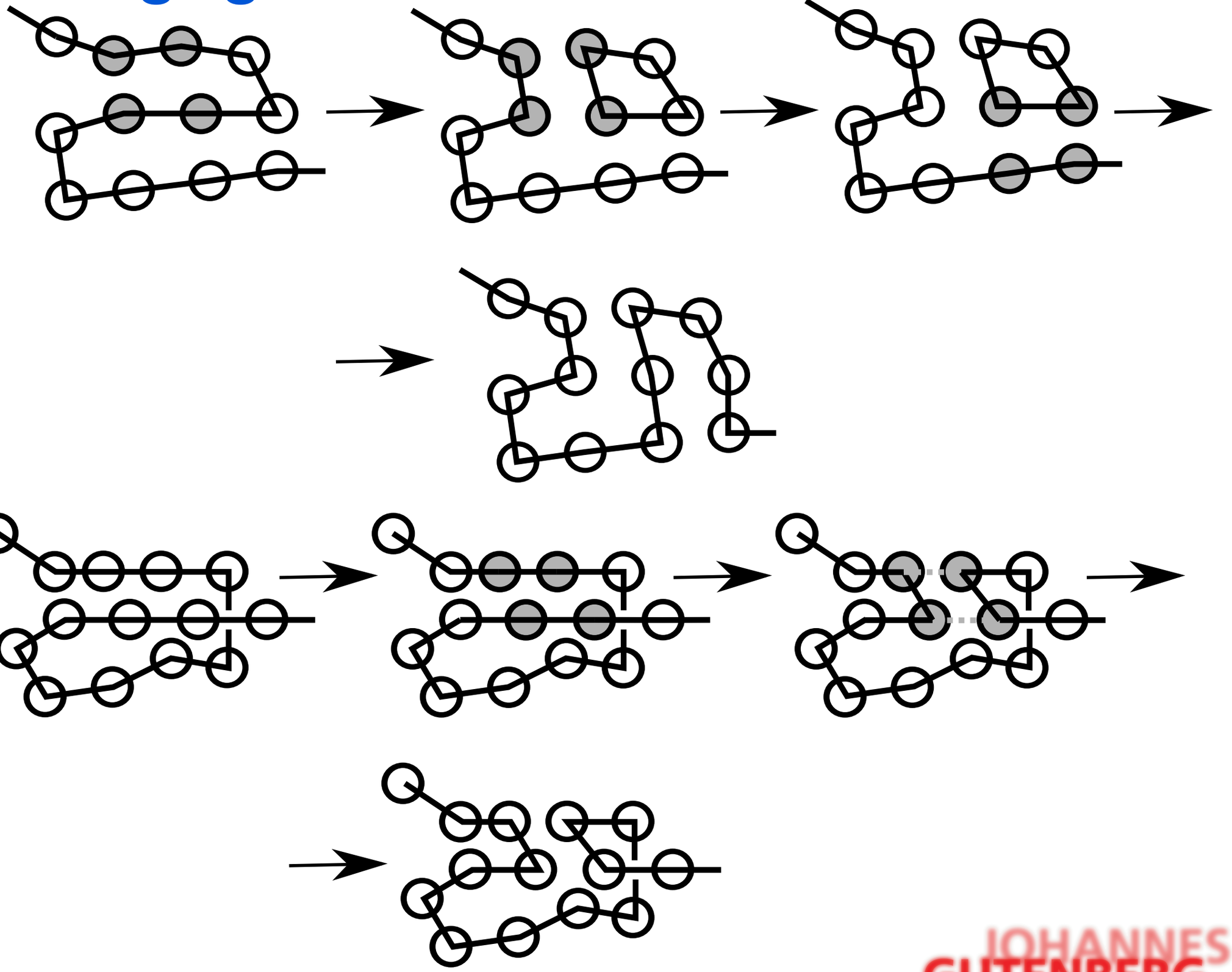
Internal rebridging

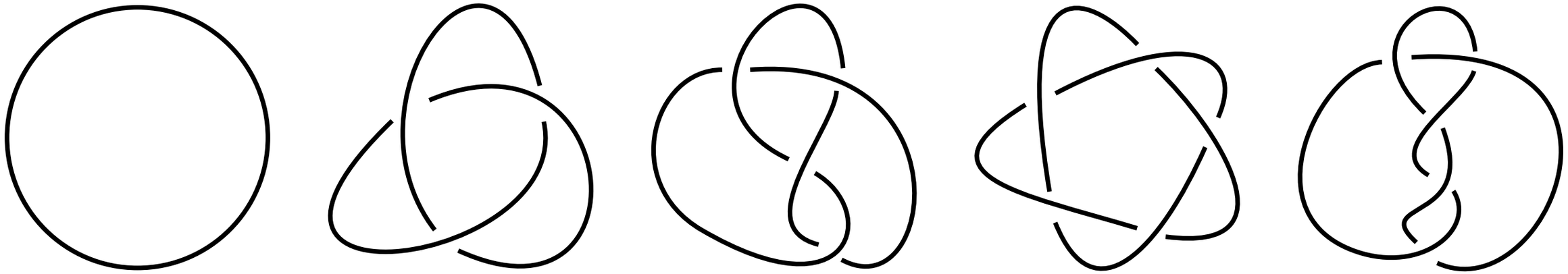


type I

type II

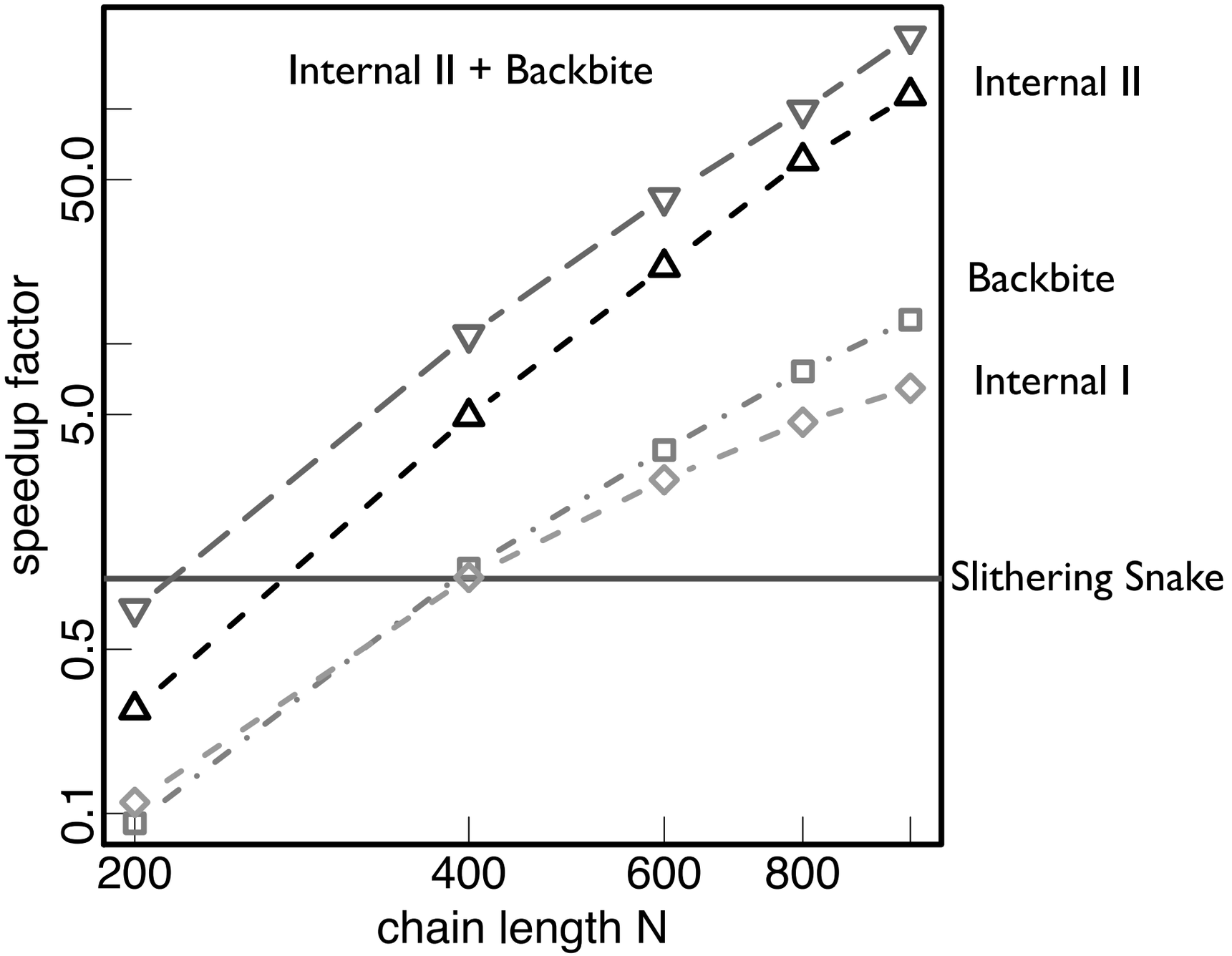
for lattice models: J.M. Deutsch, J. Chem. Phys., **106**, 8849 (1997)

Talking about topology: Knots



- topological property of closed curves in three dimensional space
- connect both ends to investigate the knottedness of open chains

Performance



- bridging faster if N > 400
- most efficient: Internal II

D. Reith and P. Virnau (submitted)

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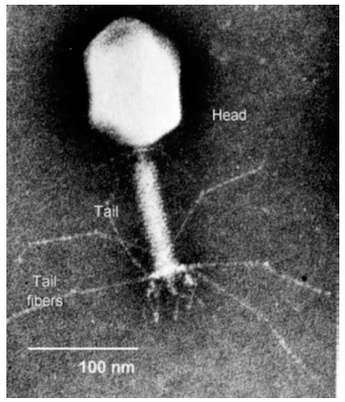
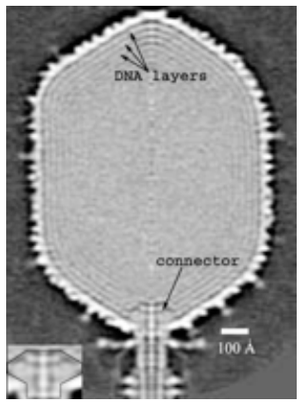
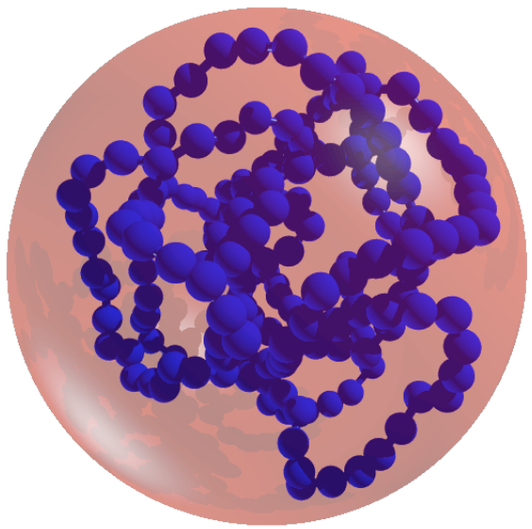
Homopolymer - motivation - experimental results





- DNA inside viral capsids is coiled up
- one end is anchored in the loading channel

- can we understand the underlying knot avoiding mechanism?



J. Arsuaga et al., PNAS **99**, 5373 (2002)
J. Arsuaga et al., PNAS **102**, 9165 (2005)

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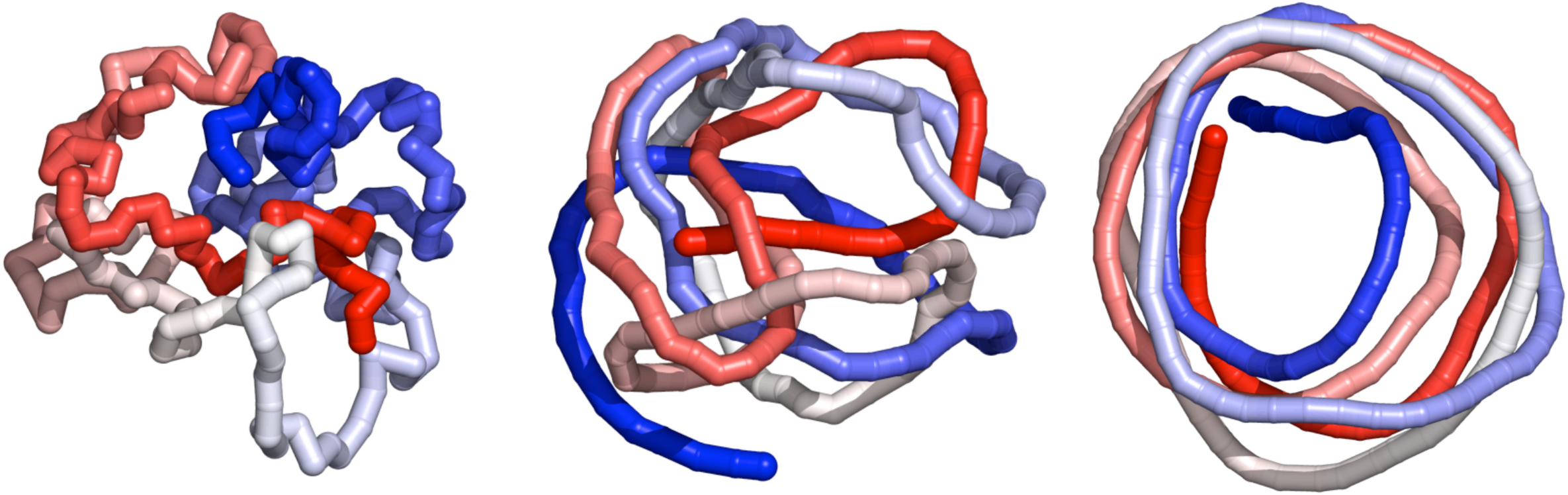
Homopolymer - results N=200



B=0 B=10 B=45

increasing bending rigidity ...

... global ordering...

D. Reith, P. Cifra and P.Virnau (in preparation)

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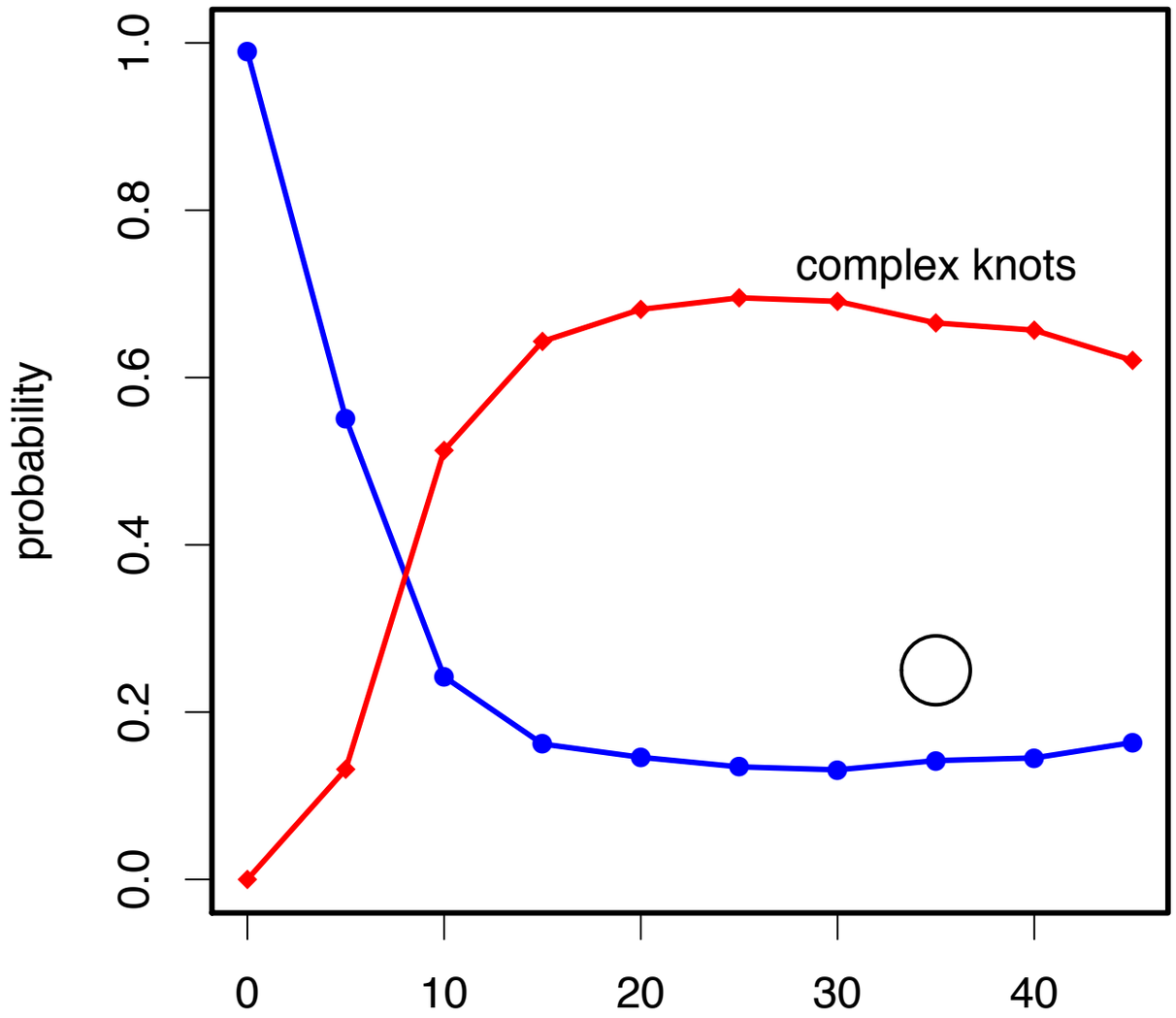
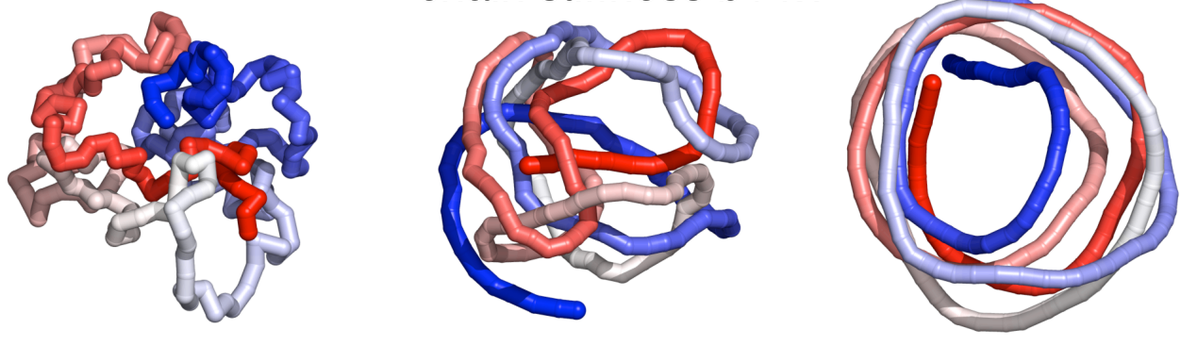
Homopolymer - results for N=200

...but semiflexible chains are „more knotted“ than flexible chains





D. Reith, P. Cifra and P.Virnau (in preparation)

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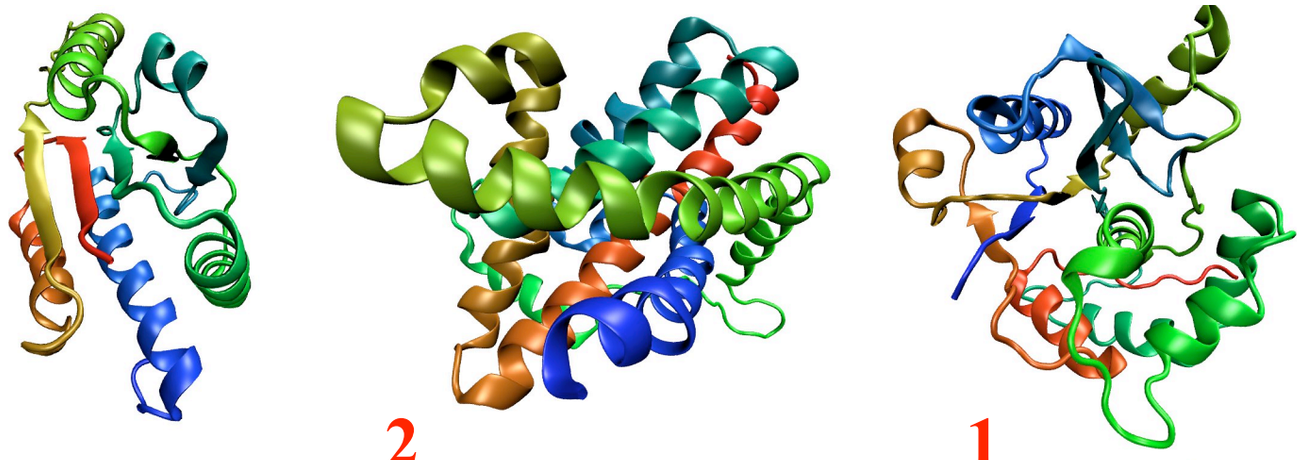
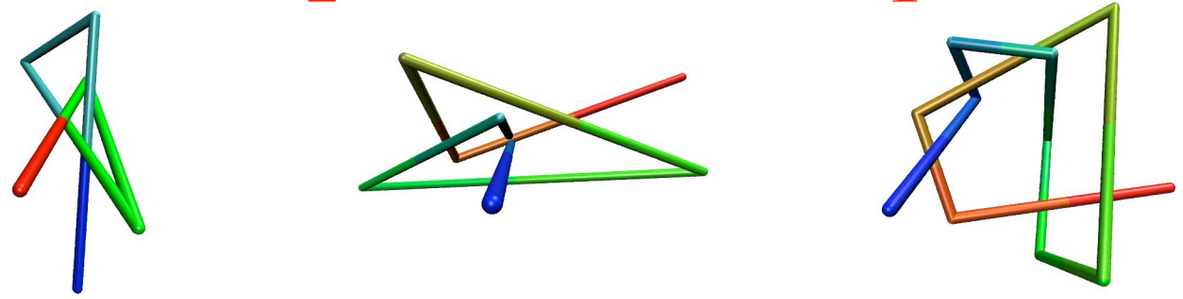
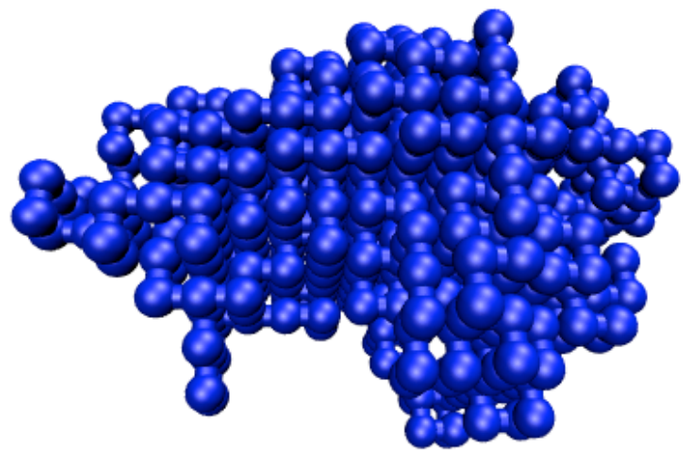
Heteropolymer - motivation



#folds: **4** **2** **1**



Probability of finding knots in proteins ~ 0.5 %



But frequent in homopolymers ~ 50 % (N=500)

P.Virnau, L.A. Mirny, and M. Kardar, PLoS Comput. Biol. **2**, e122 (2006)
P.Virnau, Y. Kantor, and M. Kardar, J. Am. Chem. Soc. **127**, 15102 (2005)

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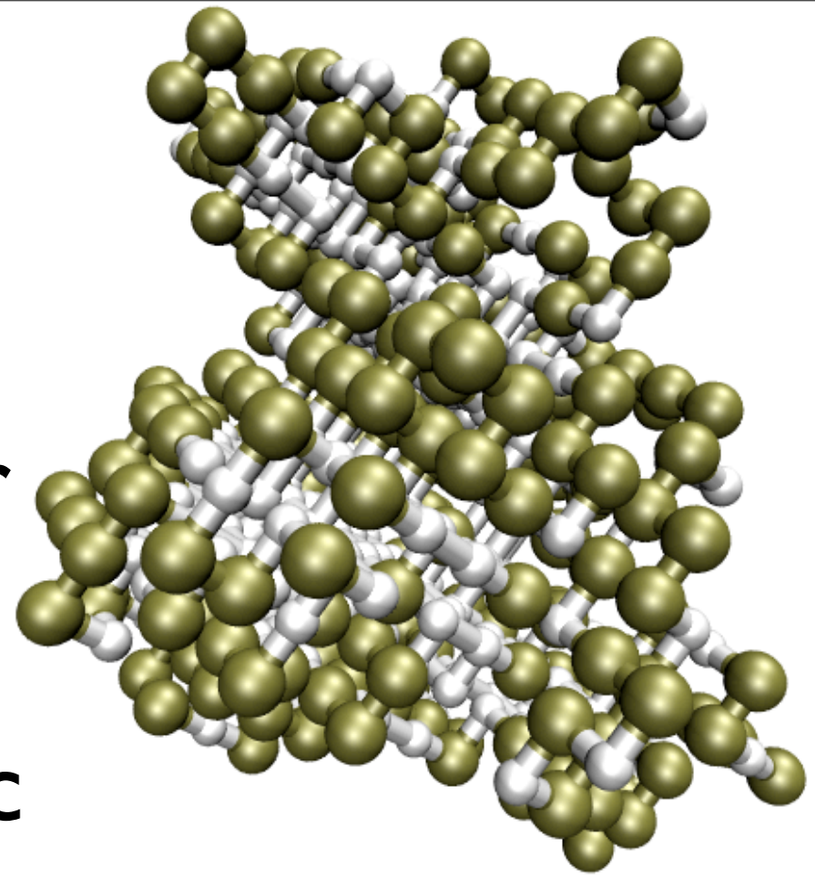
HP-model

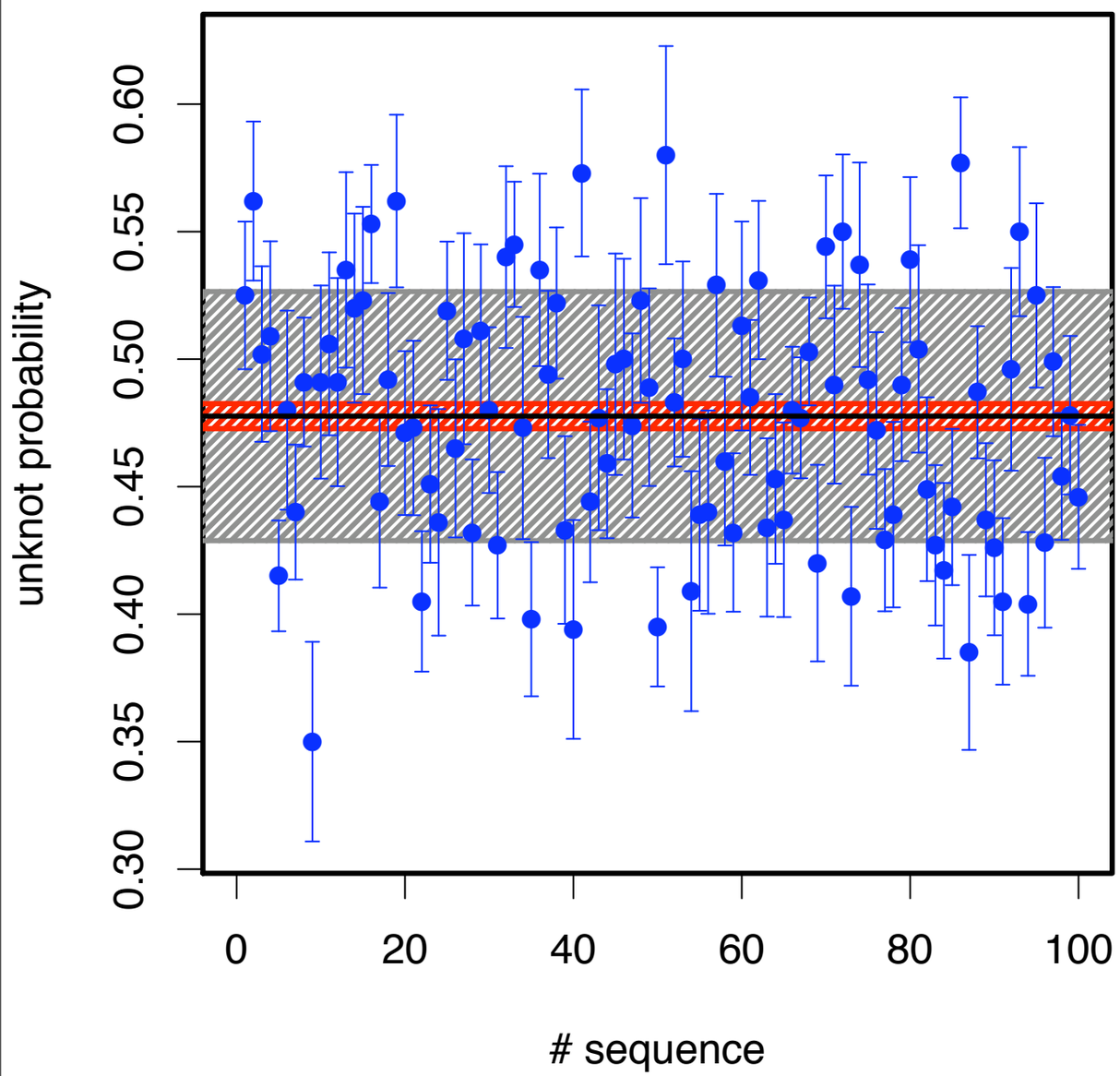


- lattice model
- excluded volume, only one monomer per site allowed
- two types of monomers: hydrophobic (H) and polar (P)
- effective interaction between neighbouring non bonded monomers:

$$\begin{aligned} \epsilon_{HH} &= -1, \\ \epsilon_{HP} &= 0, \\ \epsilon_{PP} &= 0 \end{aligned}$$

simplest toy model for coarse-grained description of protein folding

Heteropolymer - random sequences N=500



- H-P-P-H-P-H-H-H-P-P-...
- 50% H - 50 % P - like in real proteins

Results

- knotting depends on exact sequence

T. Wüst, D. Reith, and P. Virnau (in preparation)

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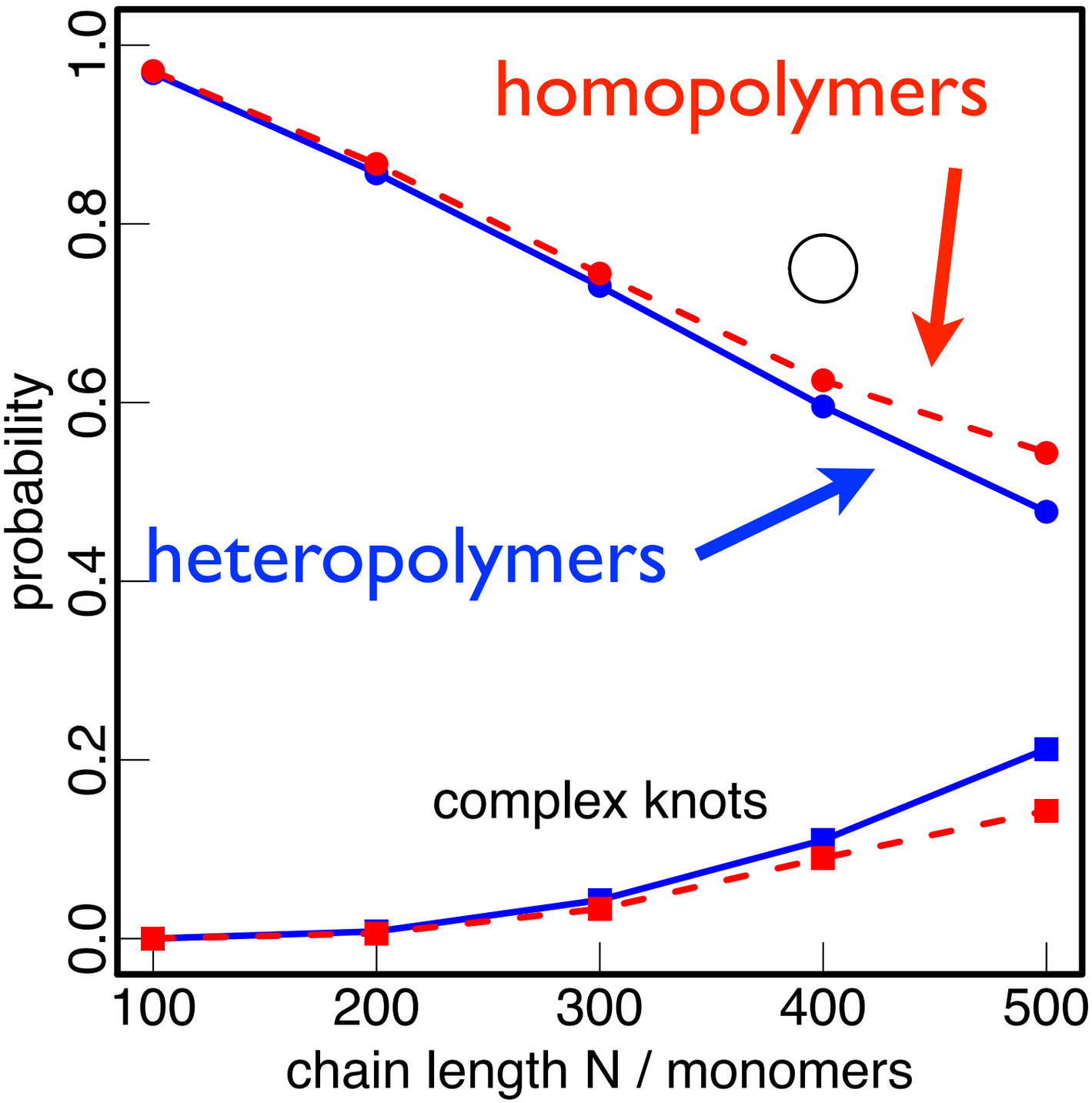
Heteropolymer - results



Knottedness in homo- and heteropolymers: similar

T. Wüst, D. Reith and P. Virnau (in preparation)

Take home messages

3 types of bridging moves: internal II most efficient

Applications:

- semiflexible homopolymers in spherical confinement: rigidity ↑ knots ↑
- random heteropolymers: knotted similar to homopolymers

Thank you!

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