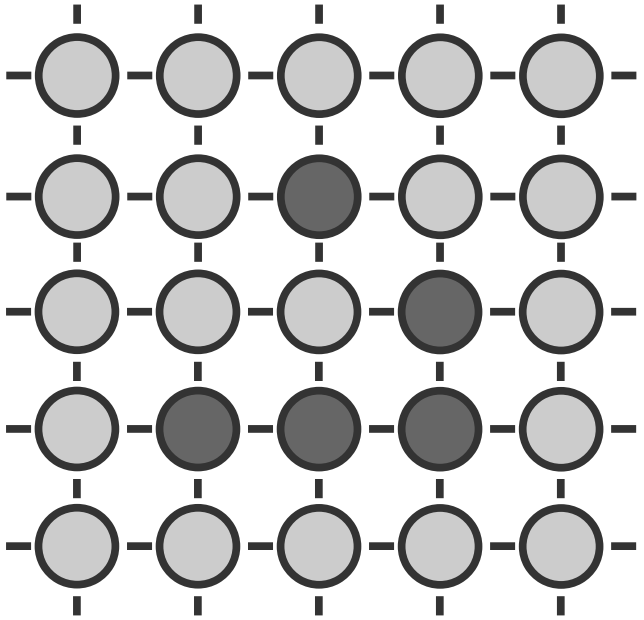
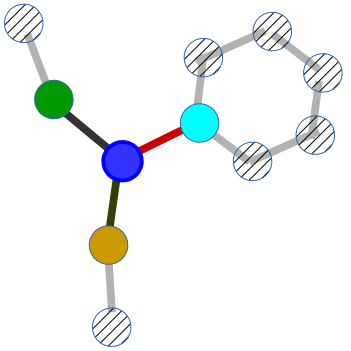
“Molecular Cellular Automata”

A parallelizable strategy for simulating *any* **active** coarse grained molecular model





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A hybrid simulation method:

a) run ordinary molecular dynamics for a short time,

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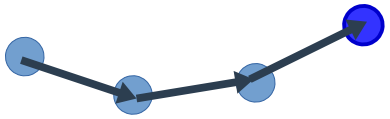

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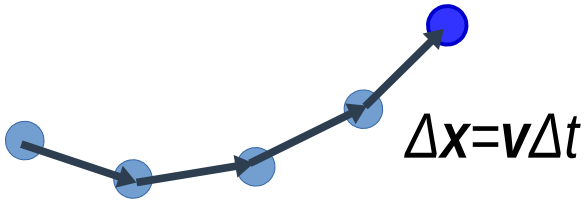

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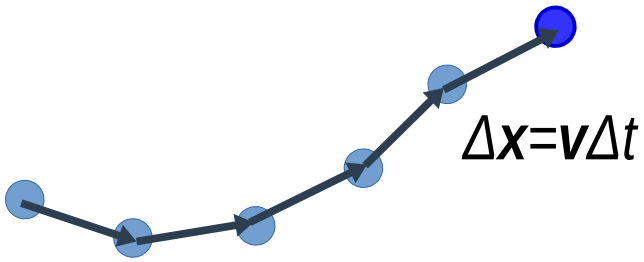

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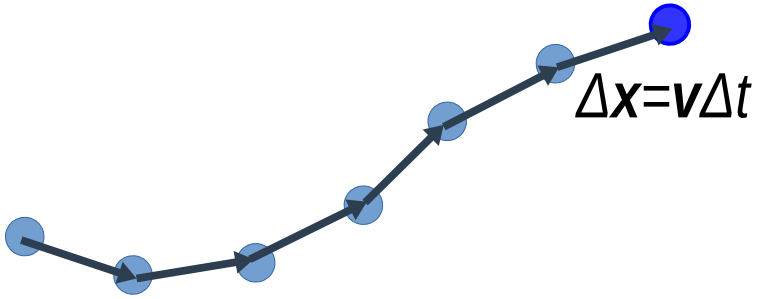

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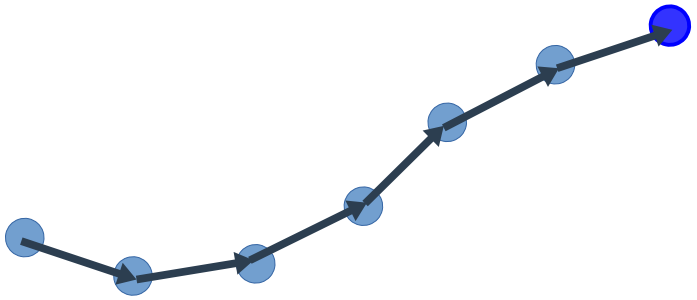

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Decisions are made ***locally***

a) At each iteration, atom types (and bond types) are modified

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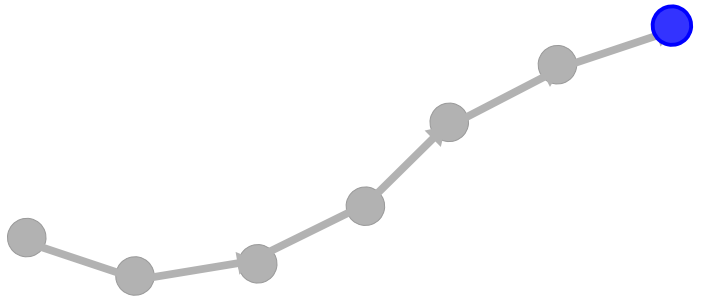

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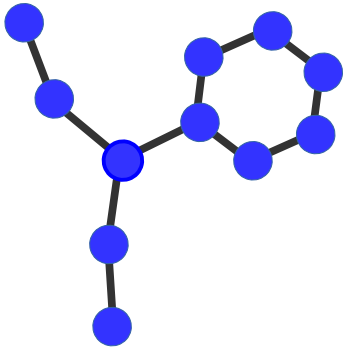

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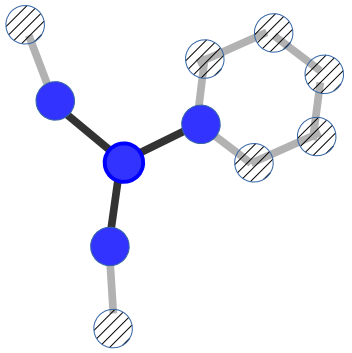

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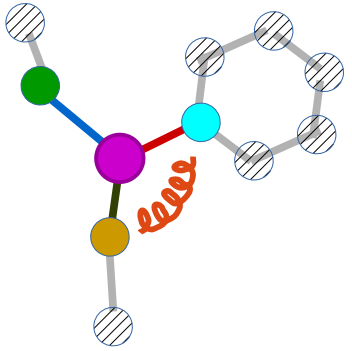

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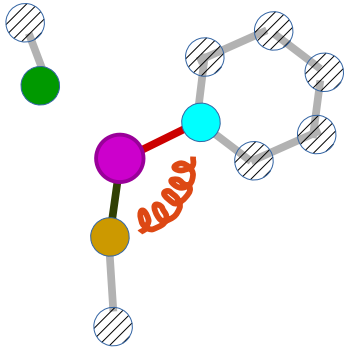

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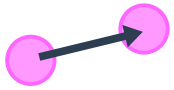

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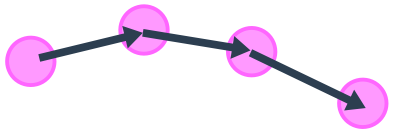

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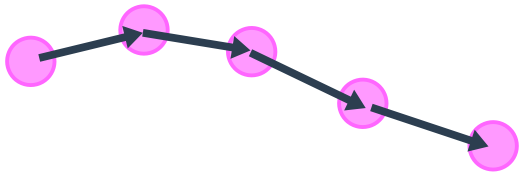

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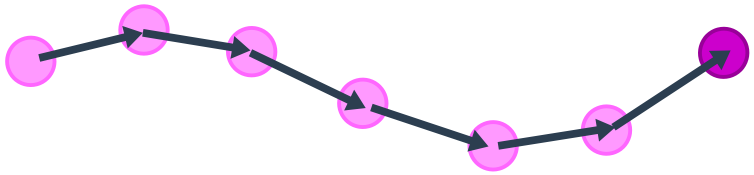
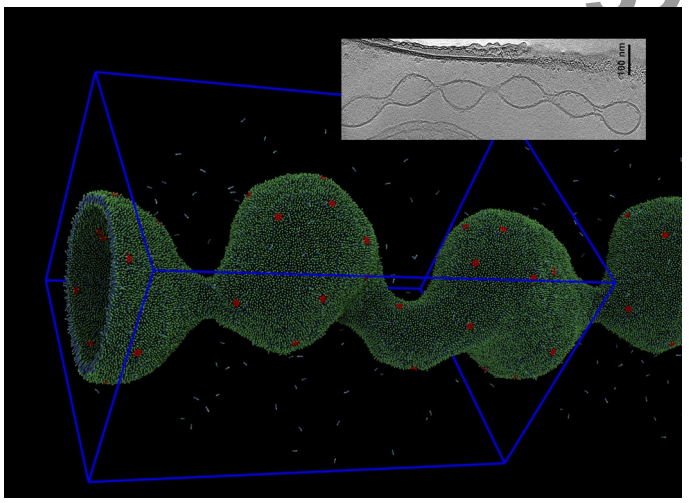
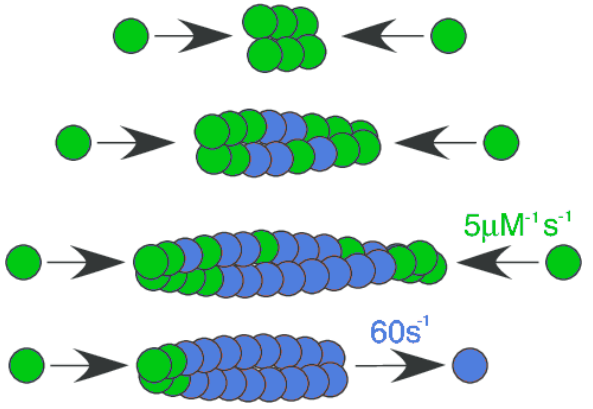


Example Uses in Biology:

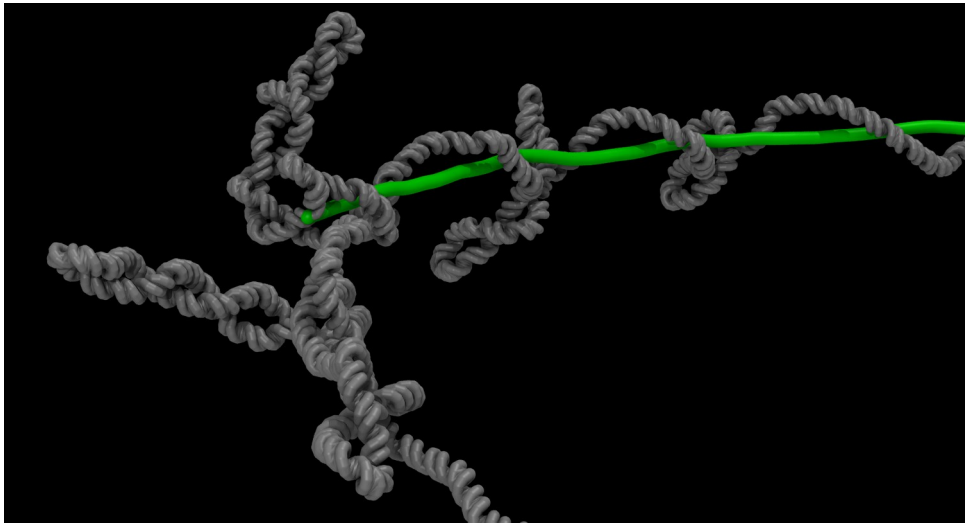
membrane trafficking



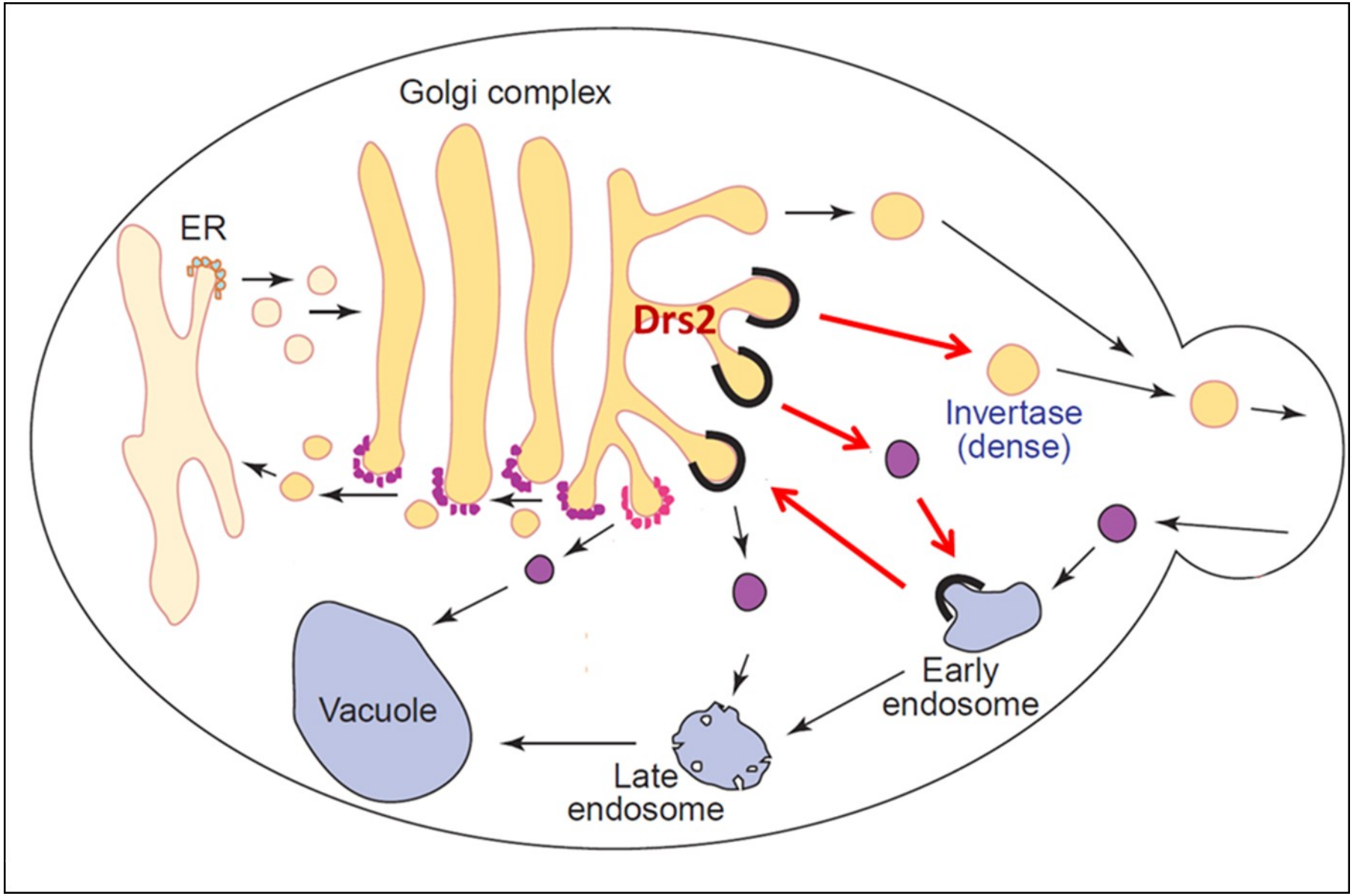
cytoskeletal filament growth dynamics



transcriptional stalling



Example: Flippase mediated membrane curvature



Graham Lab, Vanderbilt, website image

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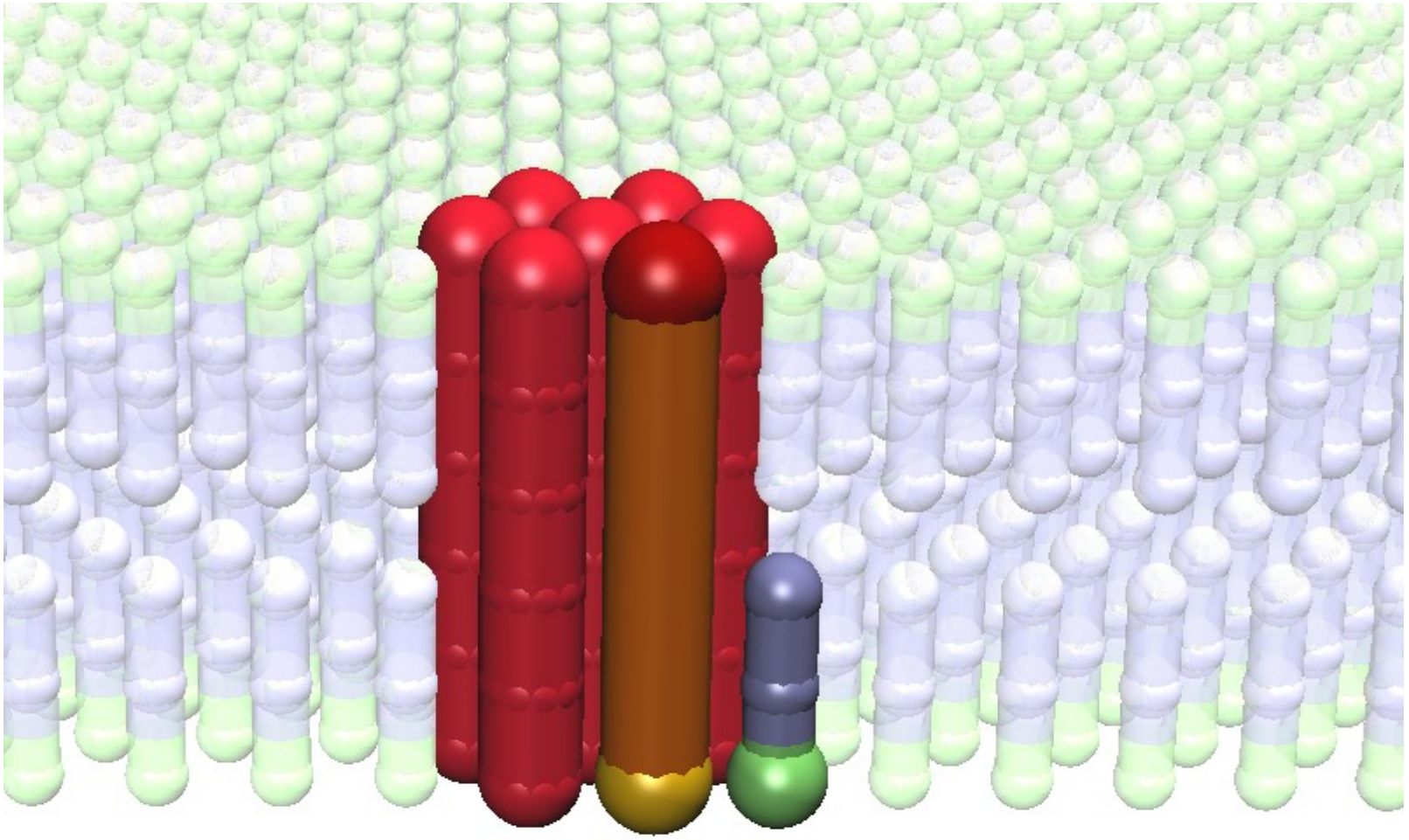

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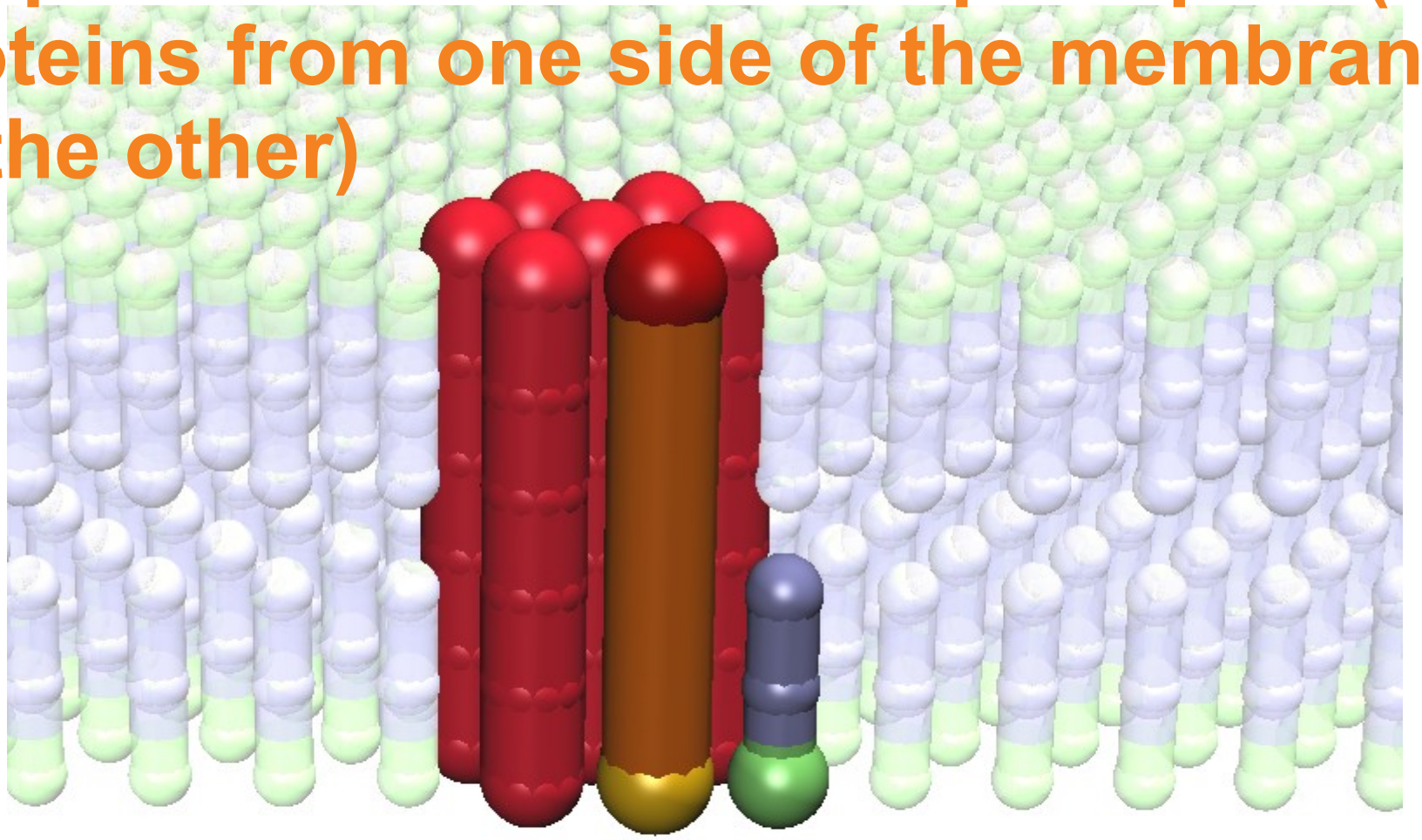
Flippase are motors which pull lipids (or proteins from one side of the membrane to the other)



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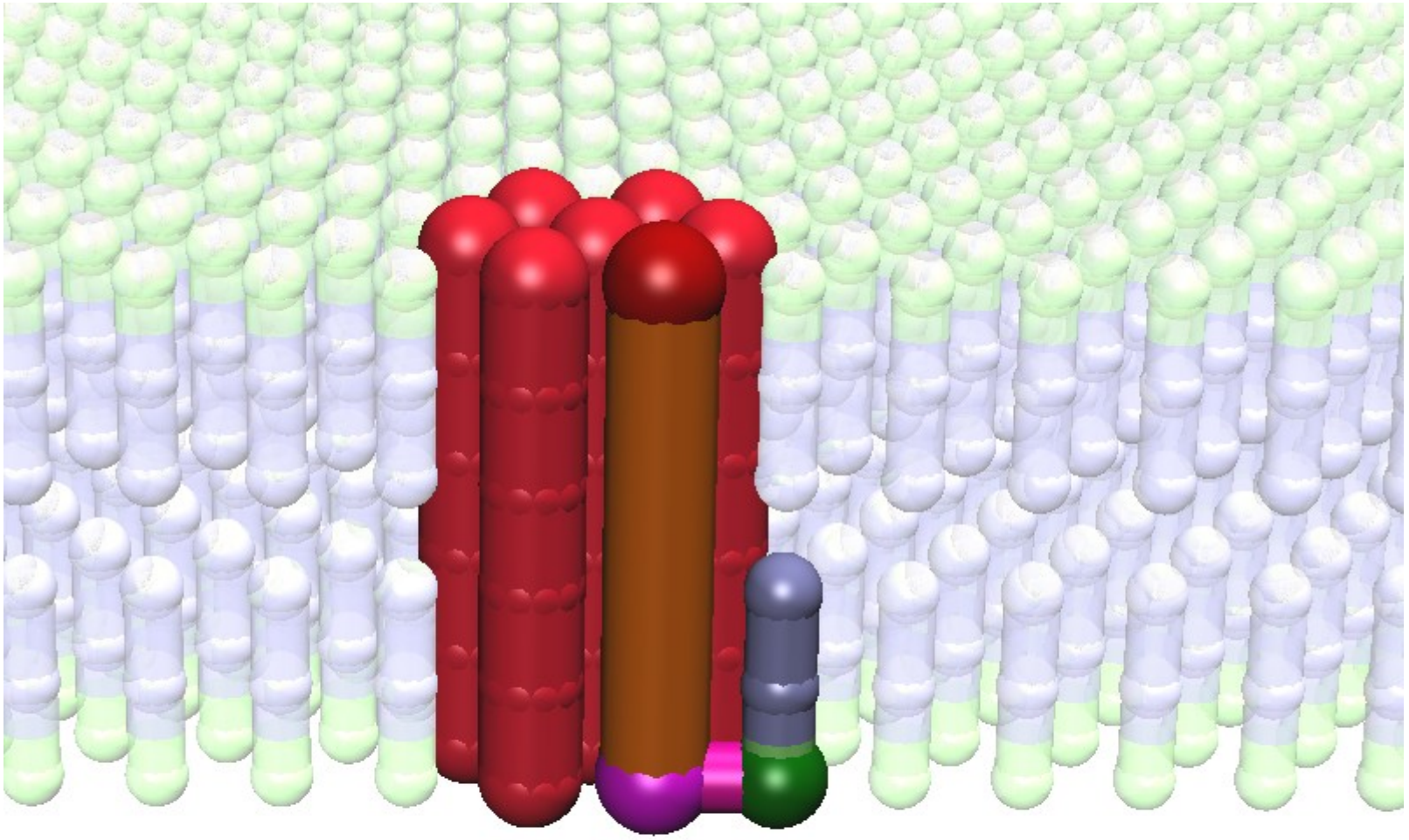

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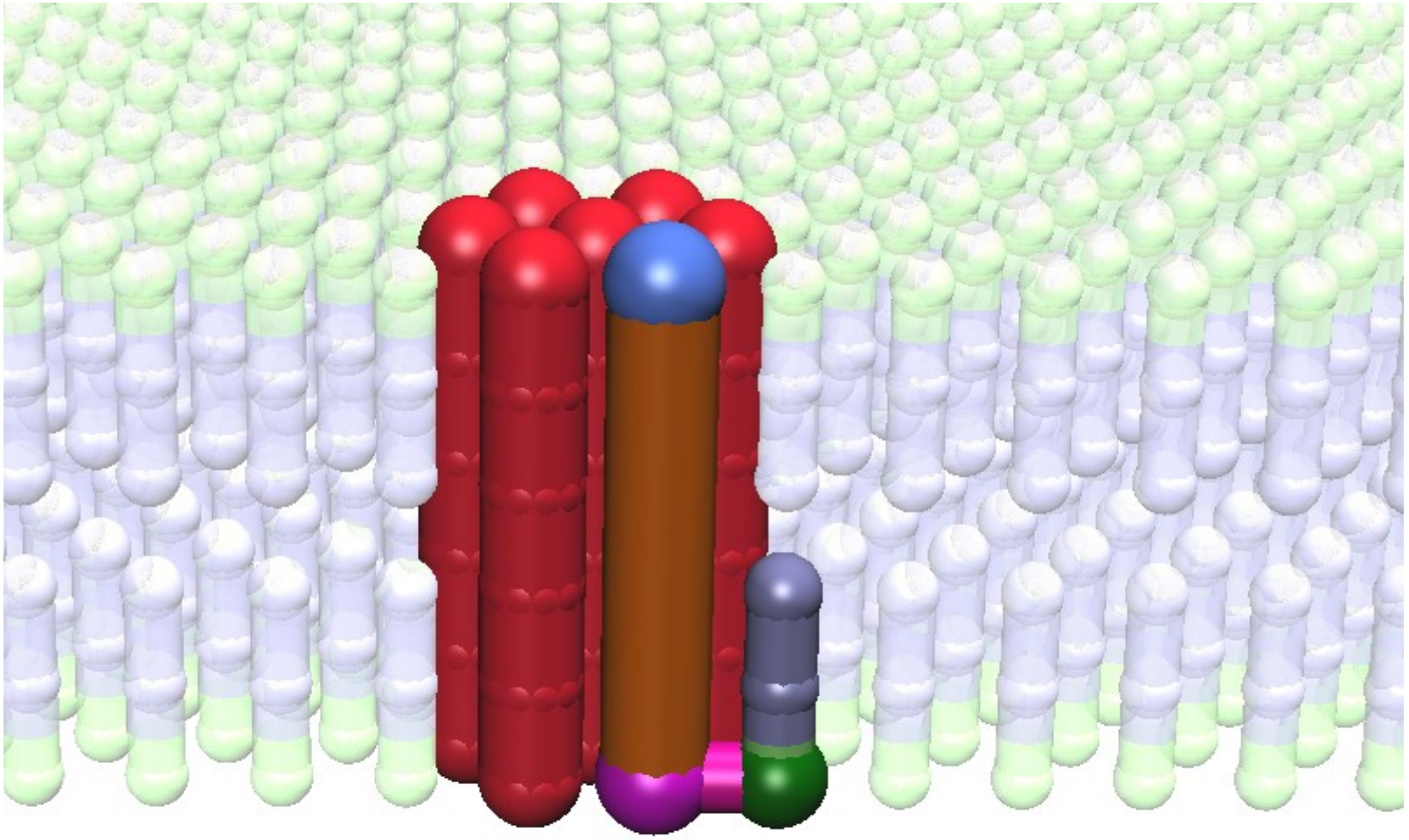

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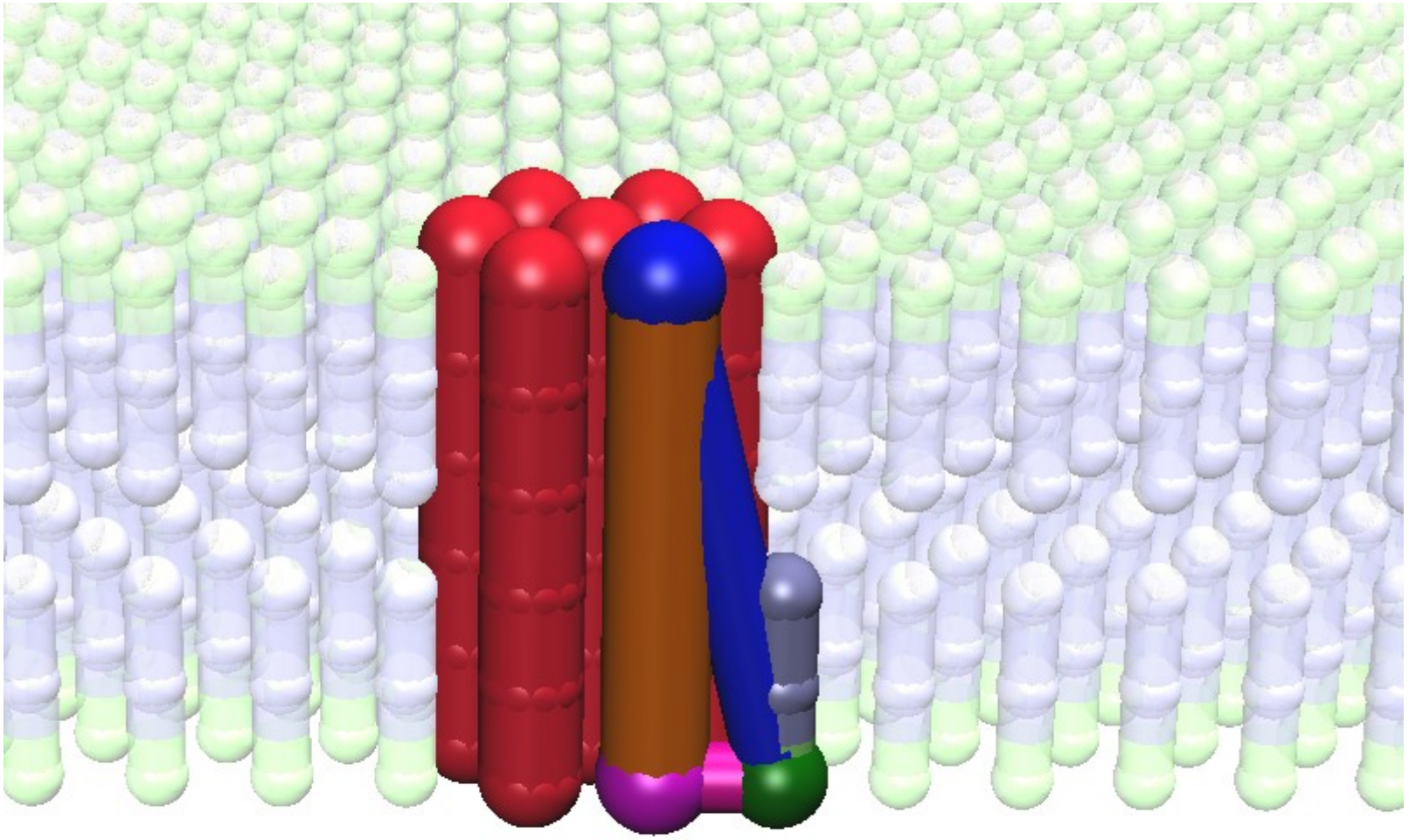

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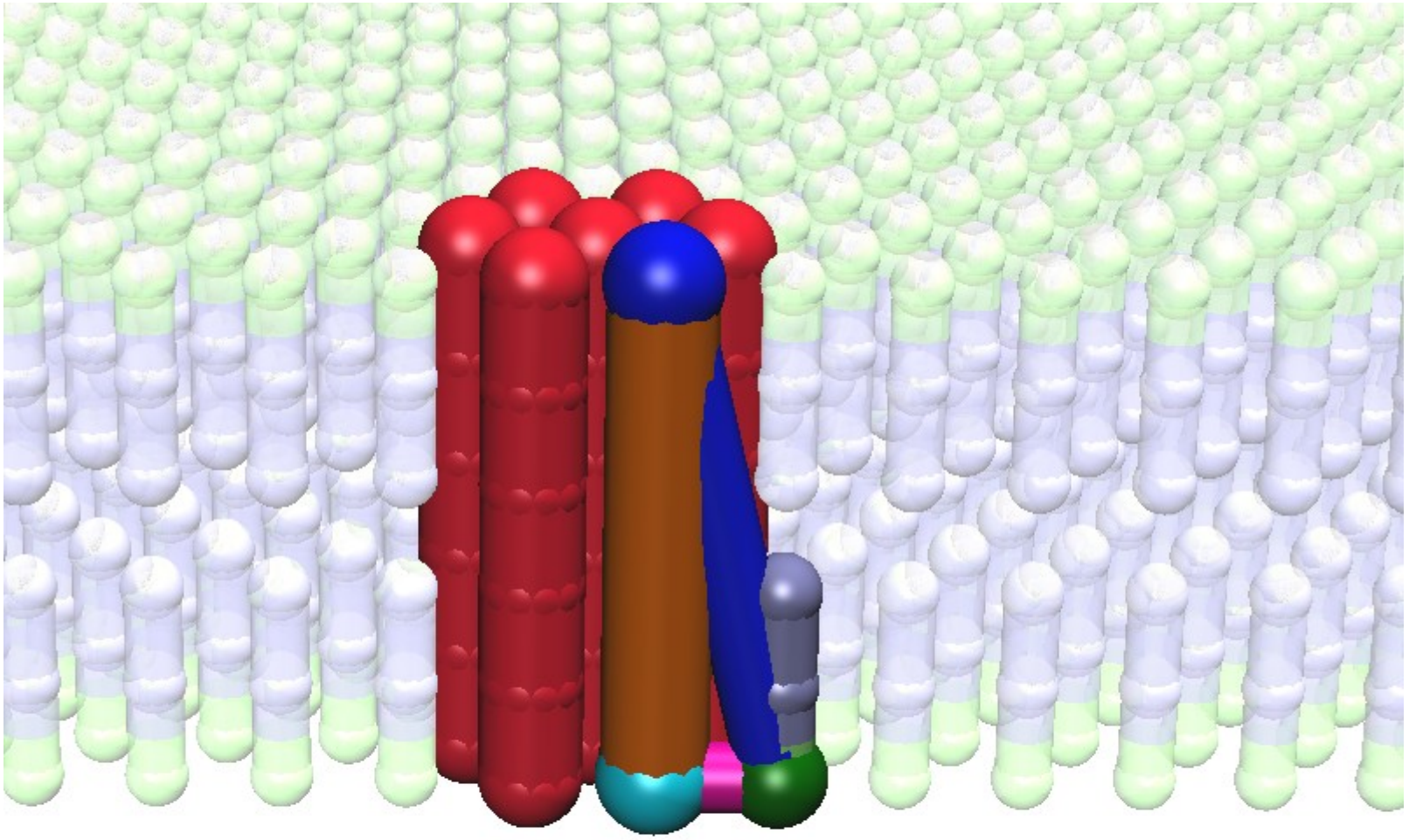

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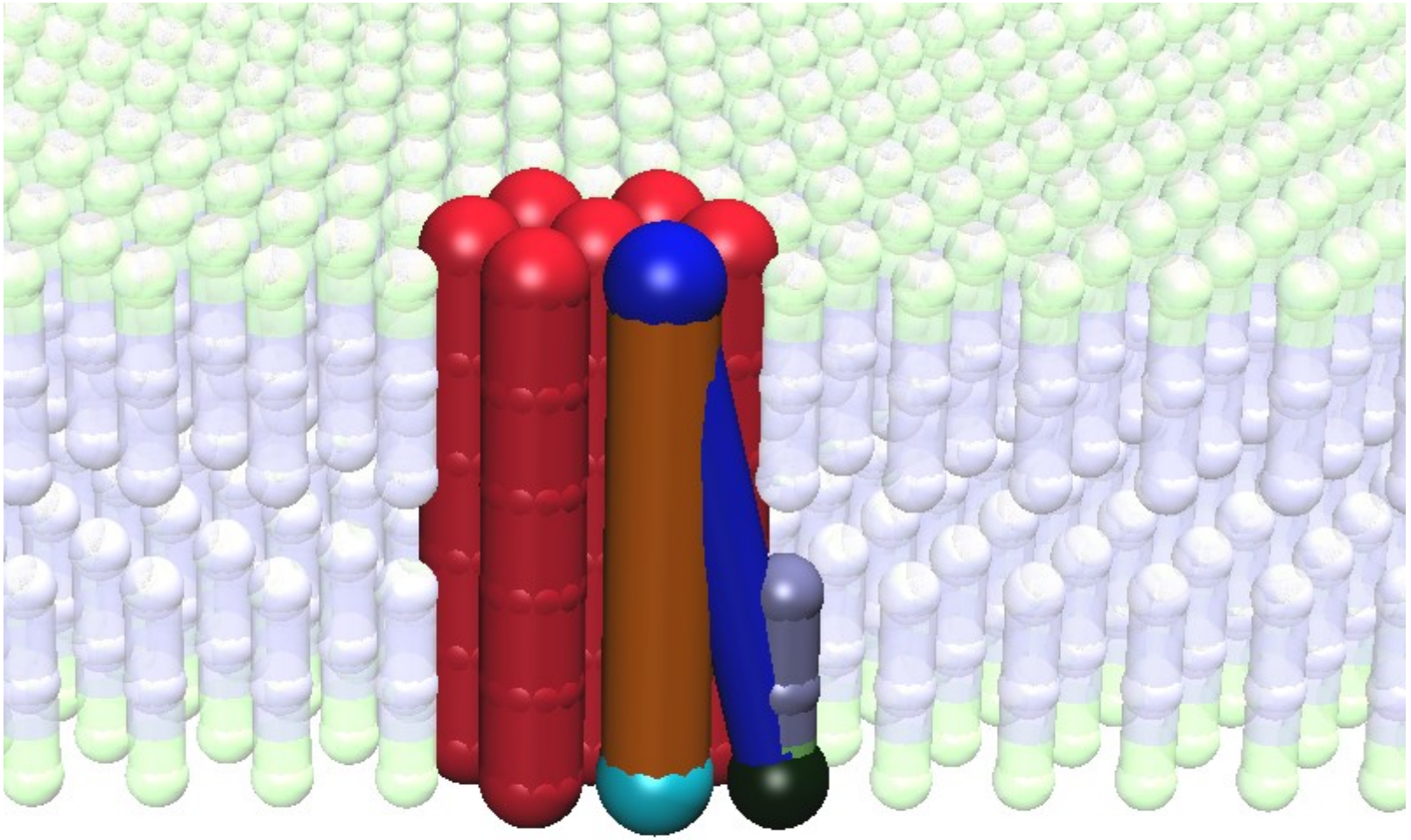

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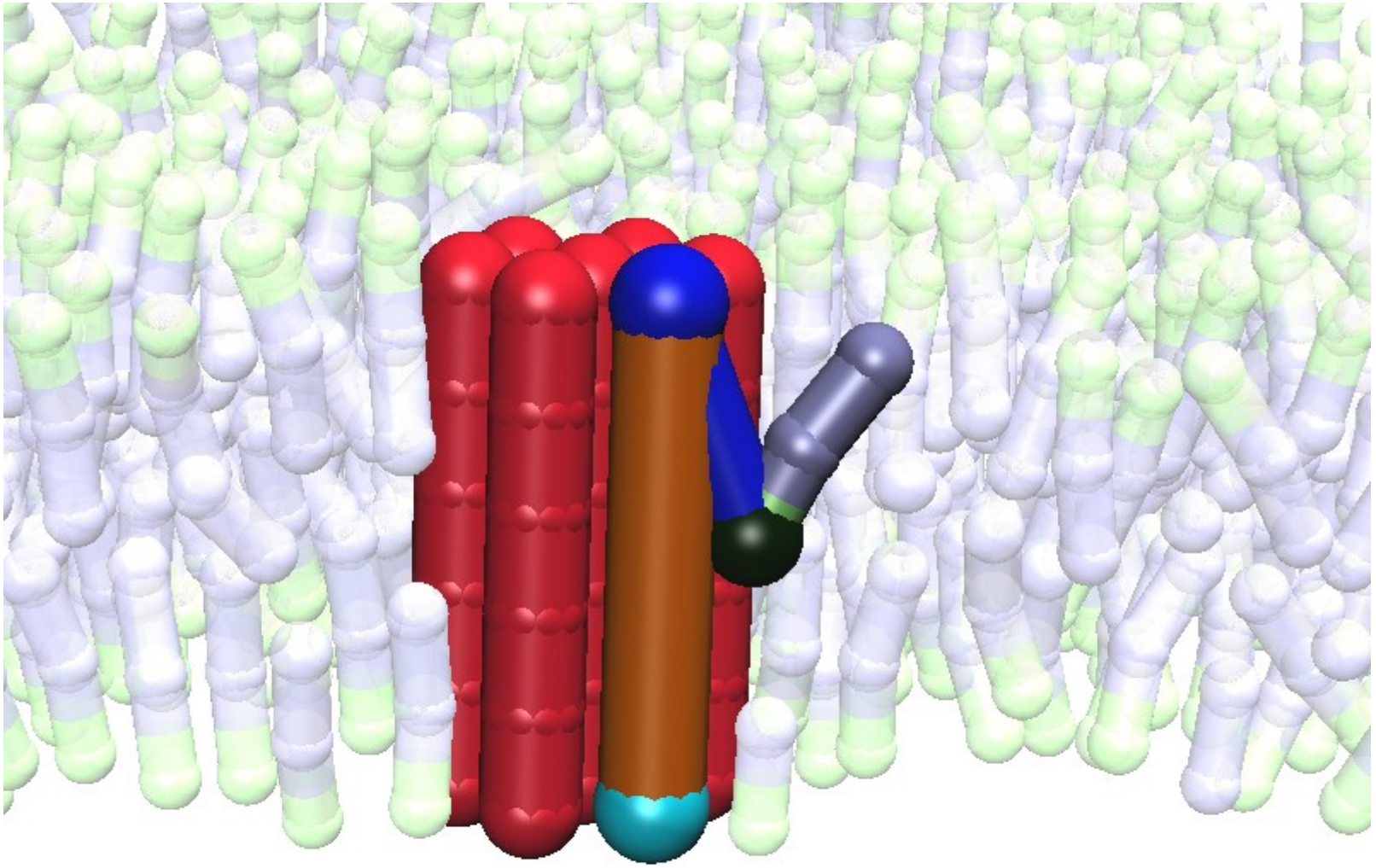

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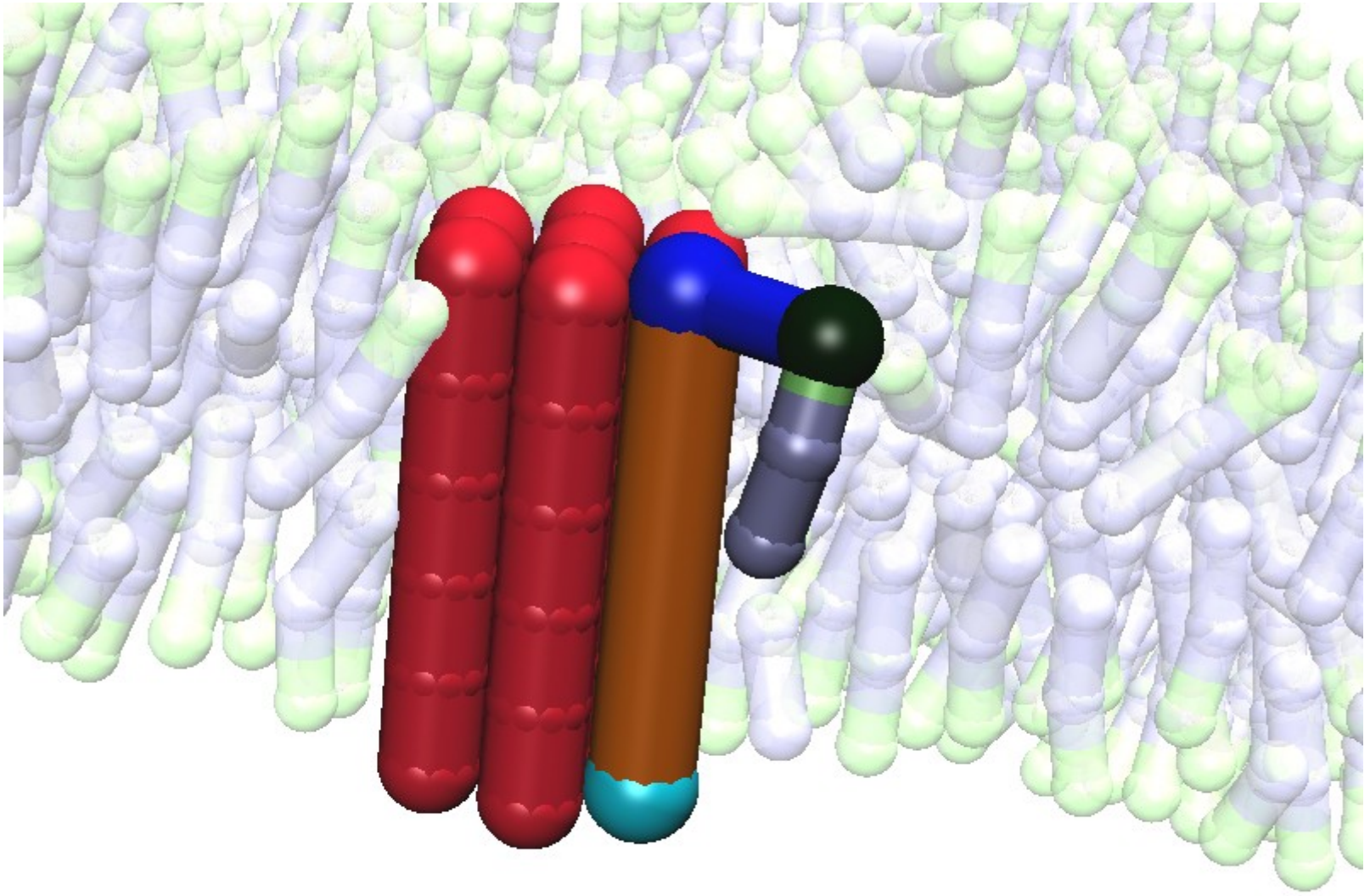

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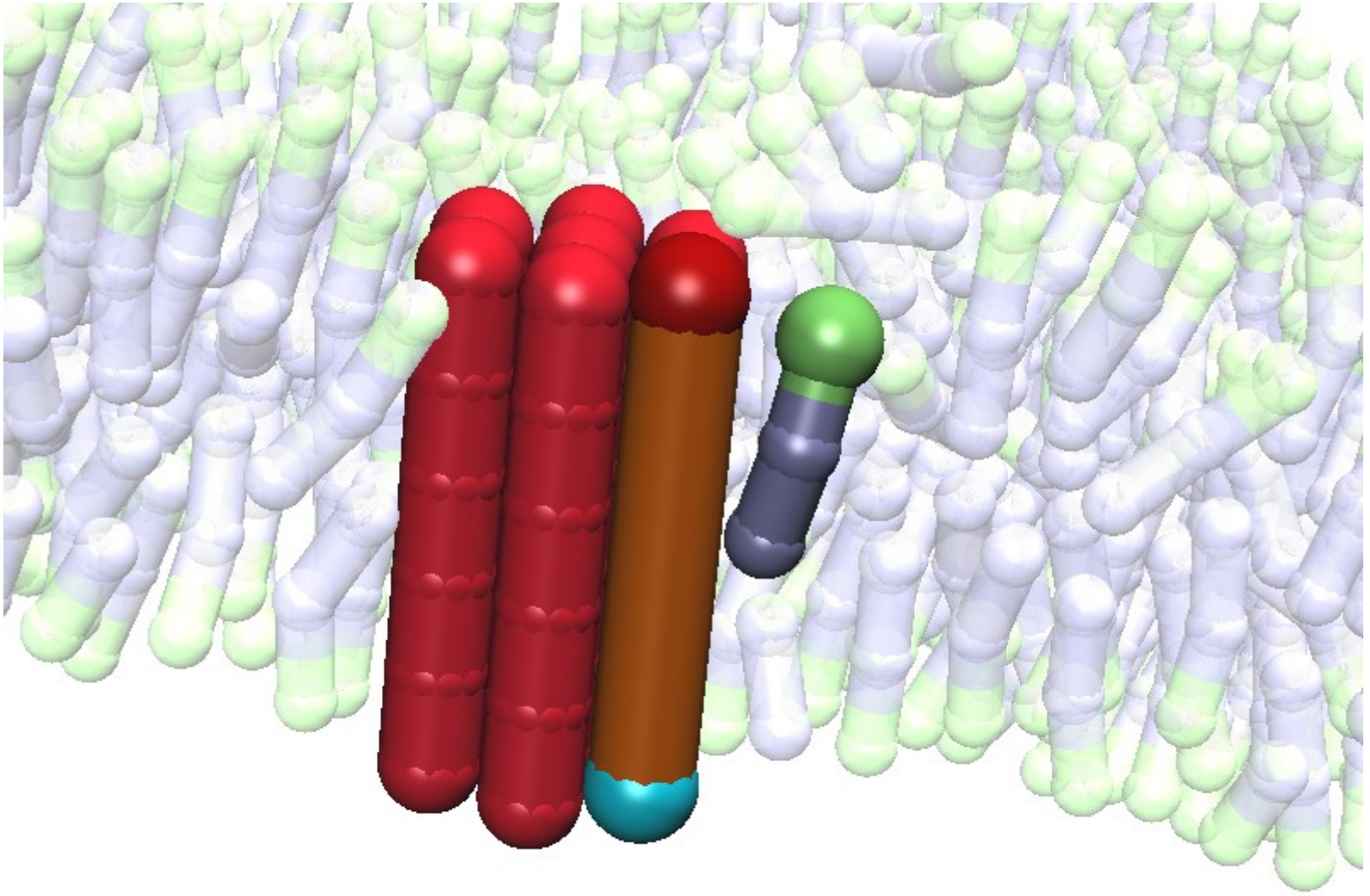

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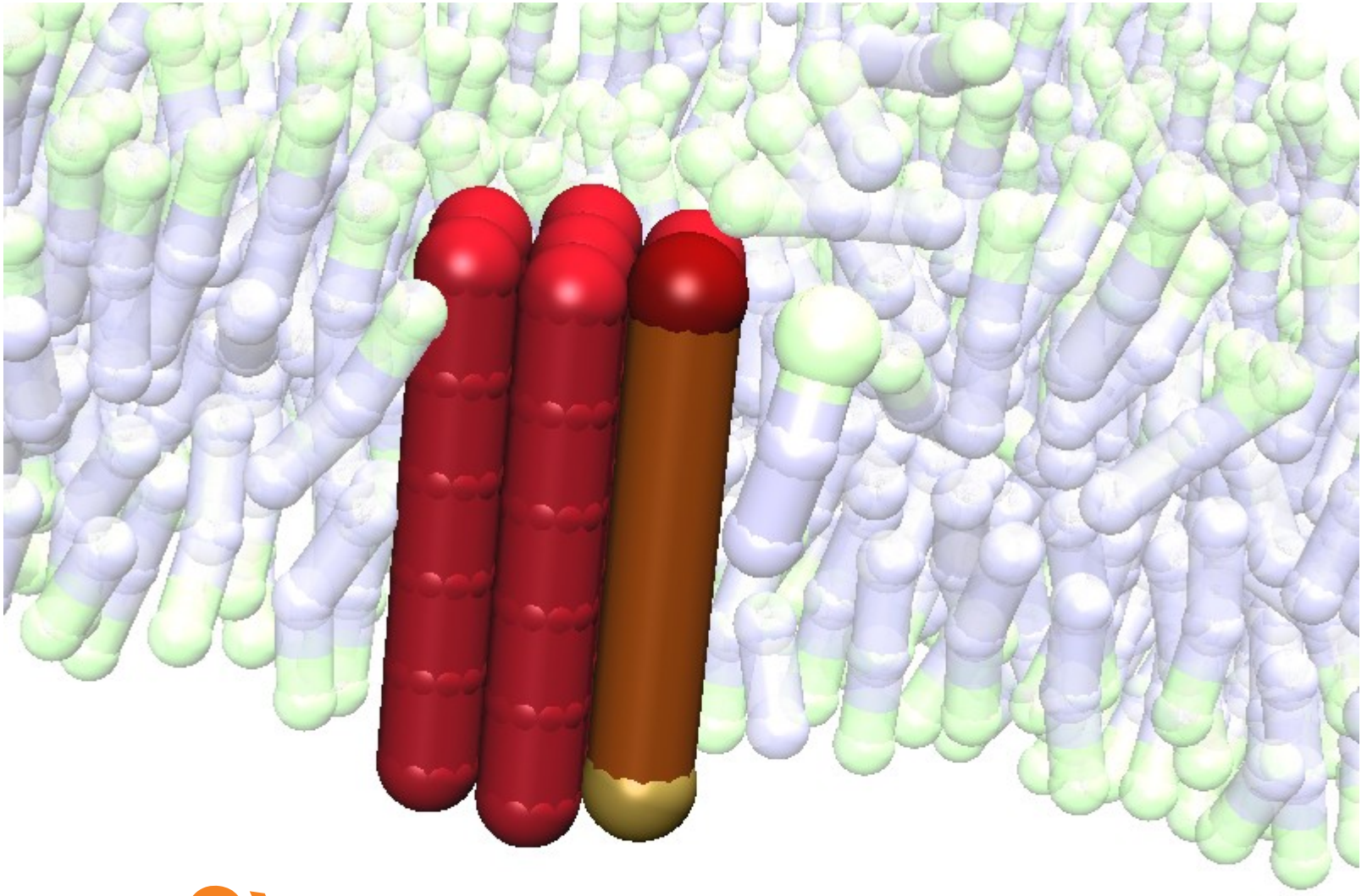

CYCLE REPEATS...

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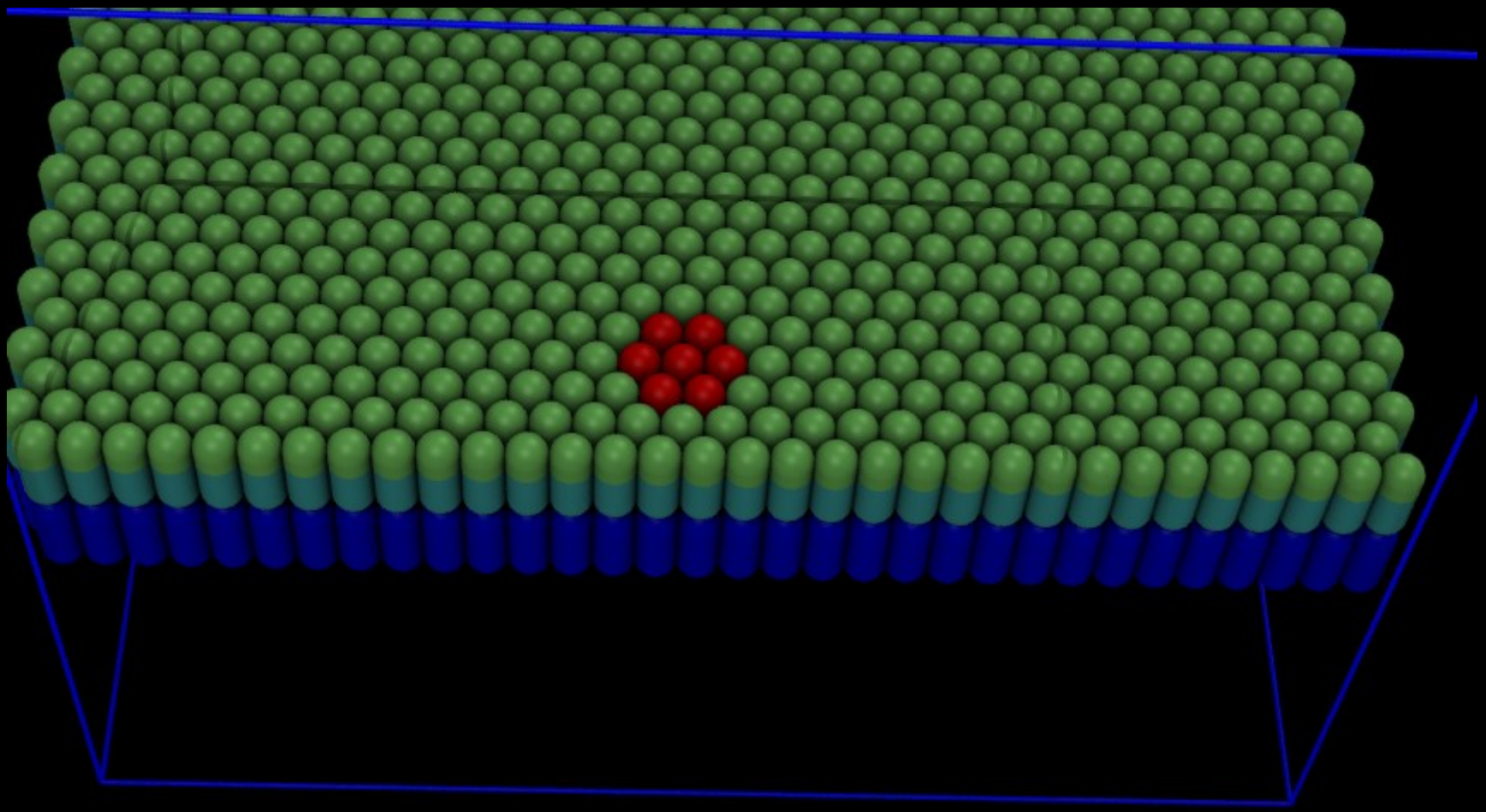

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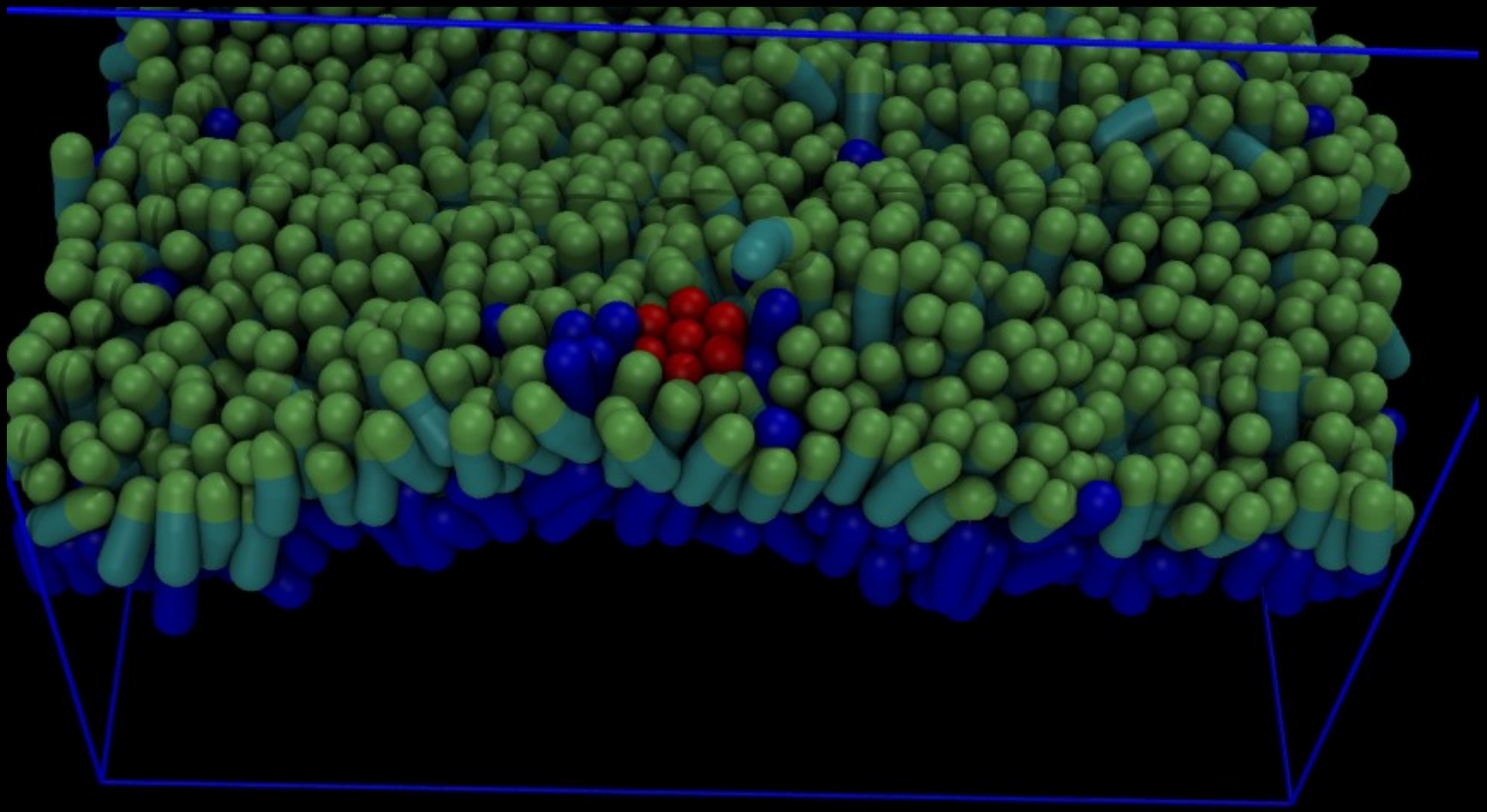

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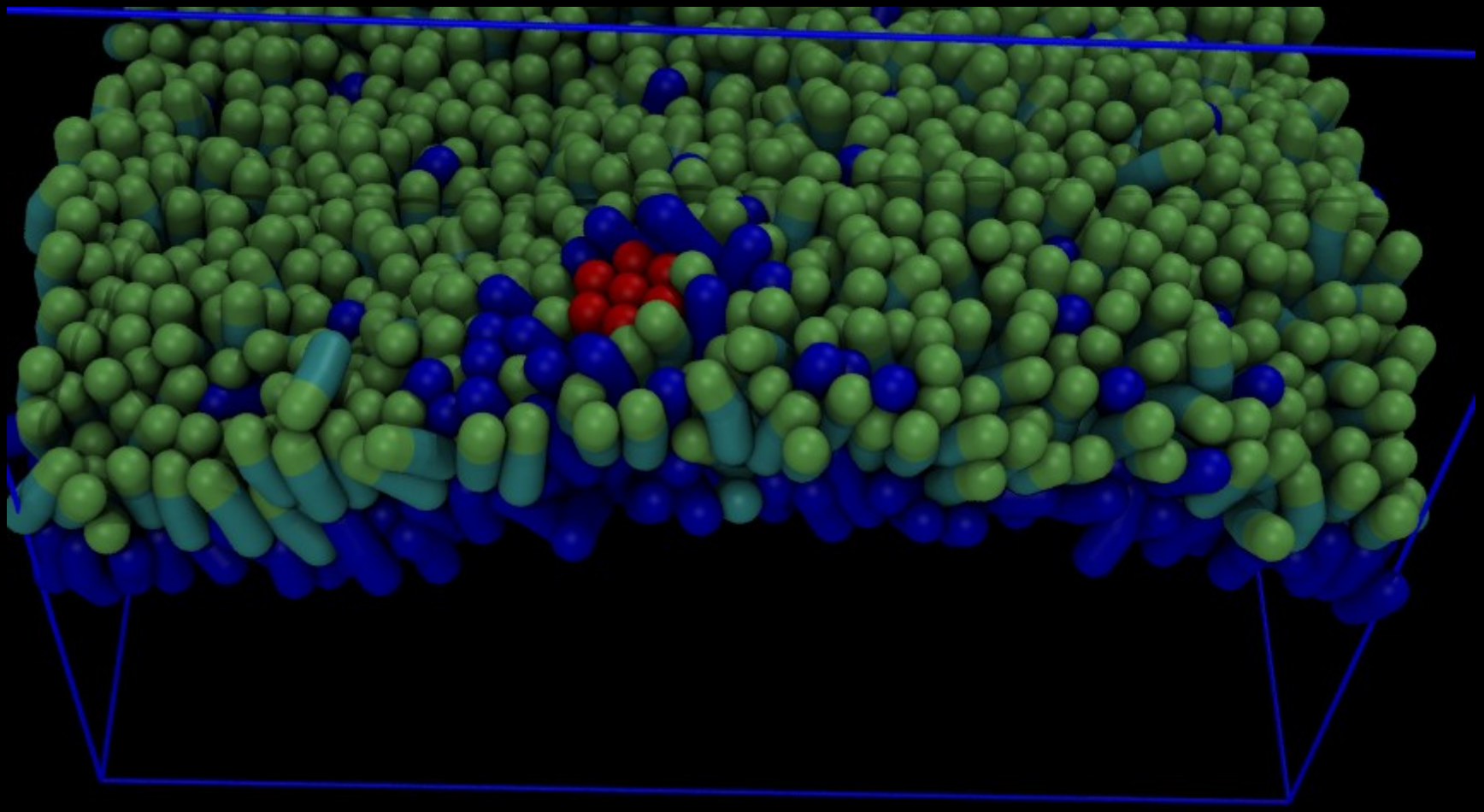

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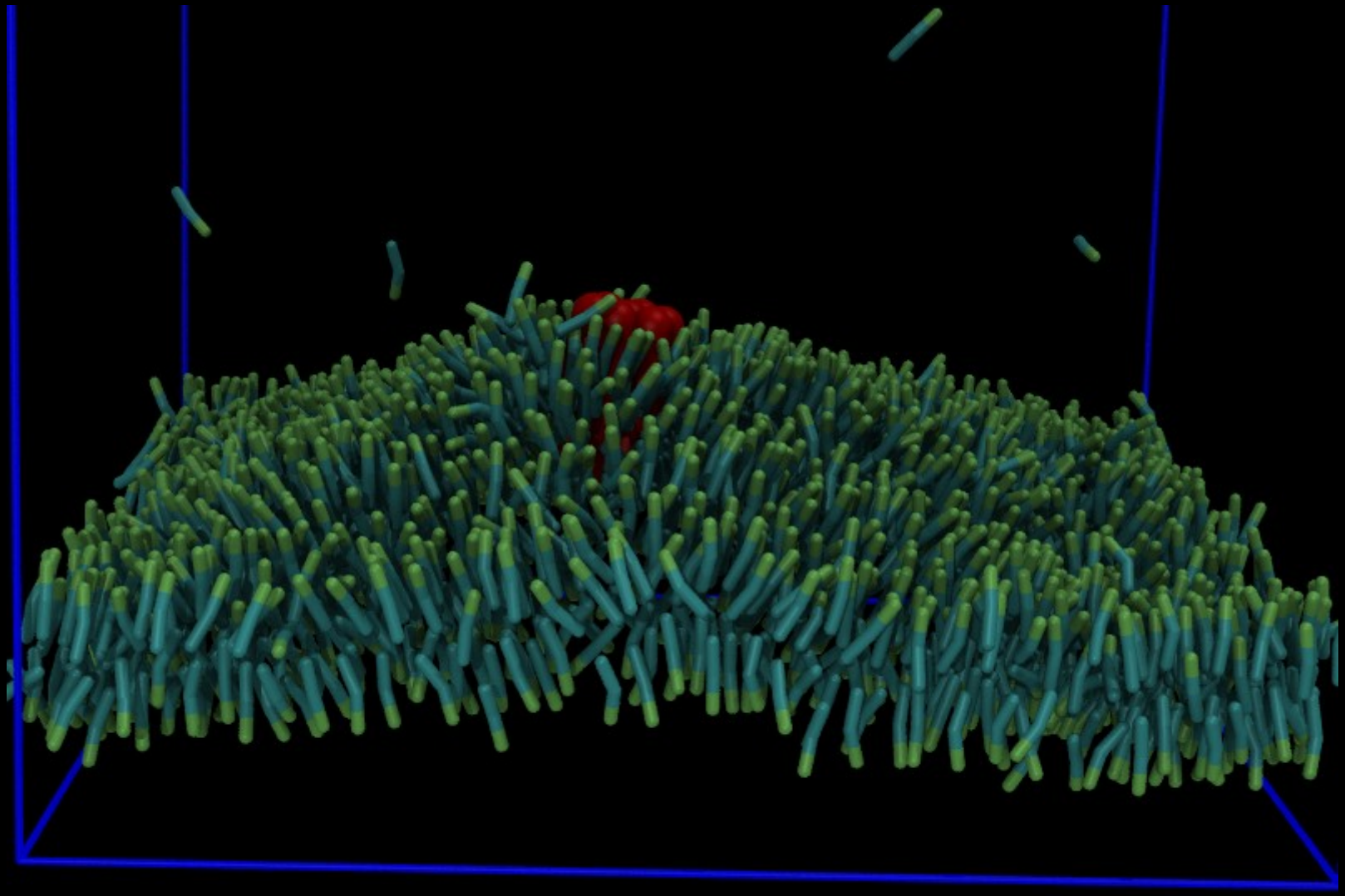

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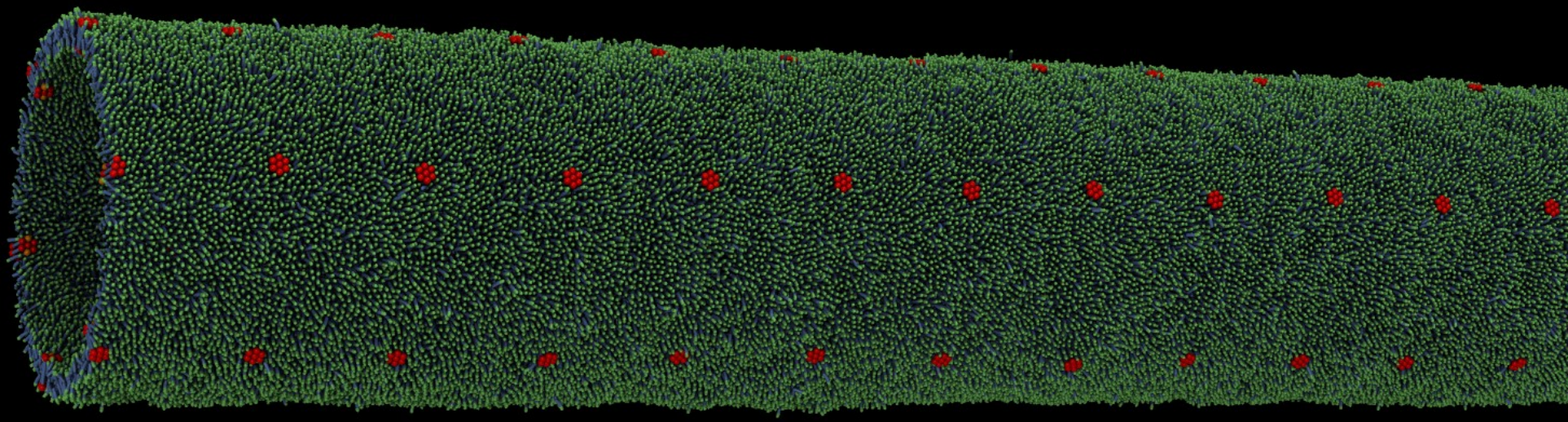

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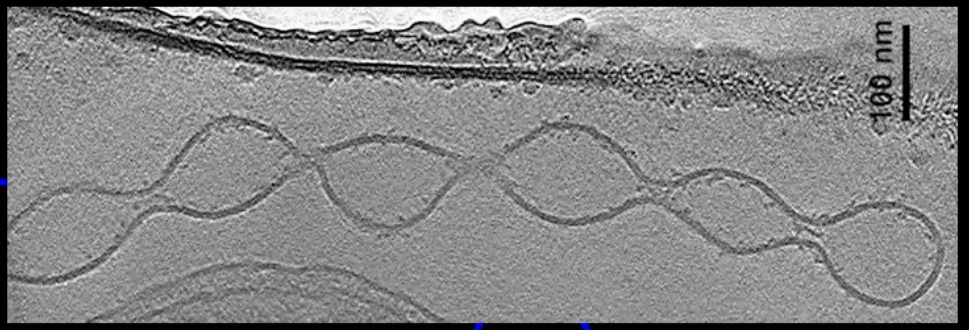
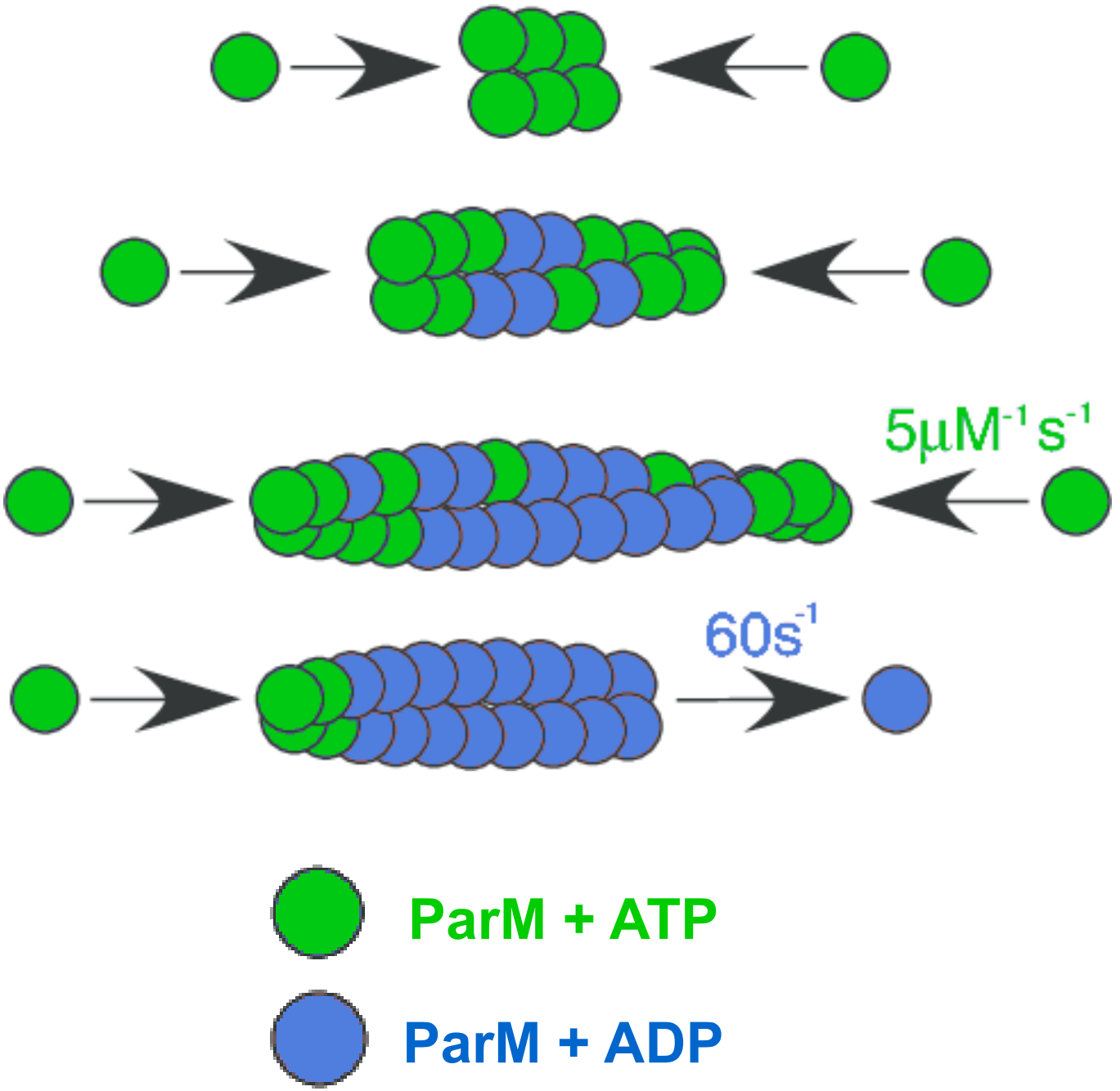


P. Subramanian, … G.J.Jensen, BioRXiv(2016)

SEE: https://www.youtube.com/watch?v=0cuEeCdyokU

Example 2: Dynamic Instabilty of ParM



Garner, …, Mullins, Science (2004)

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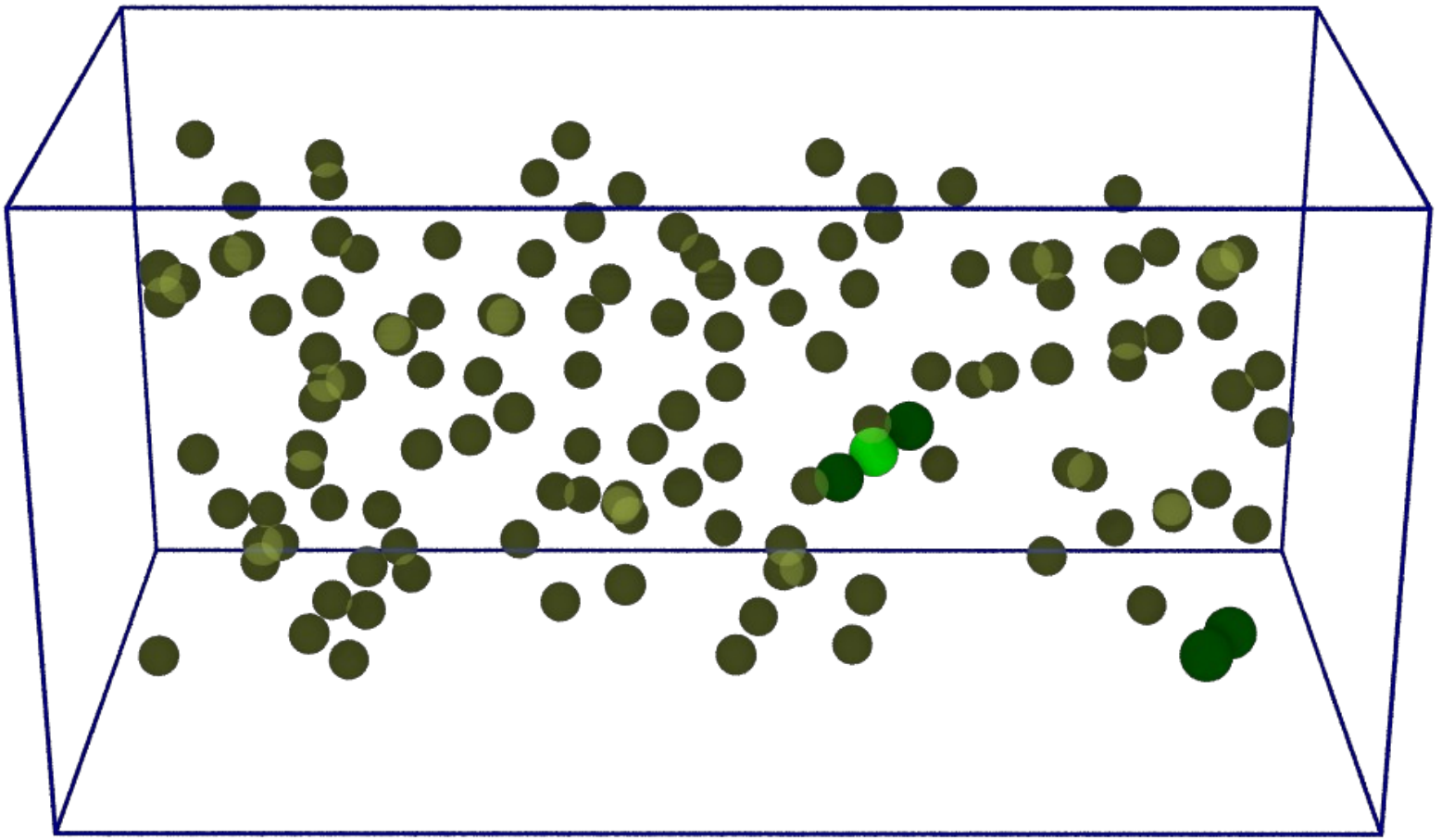

ParM + ATP

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Garner, …, Mullins, Science (2004)

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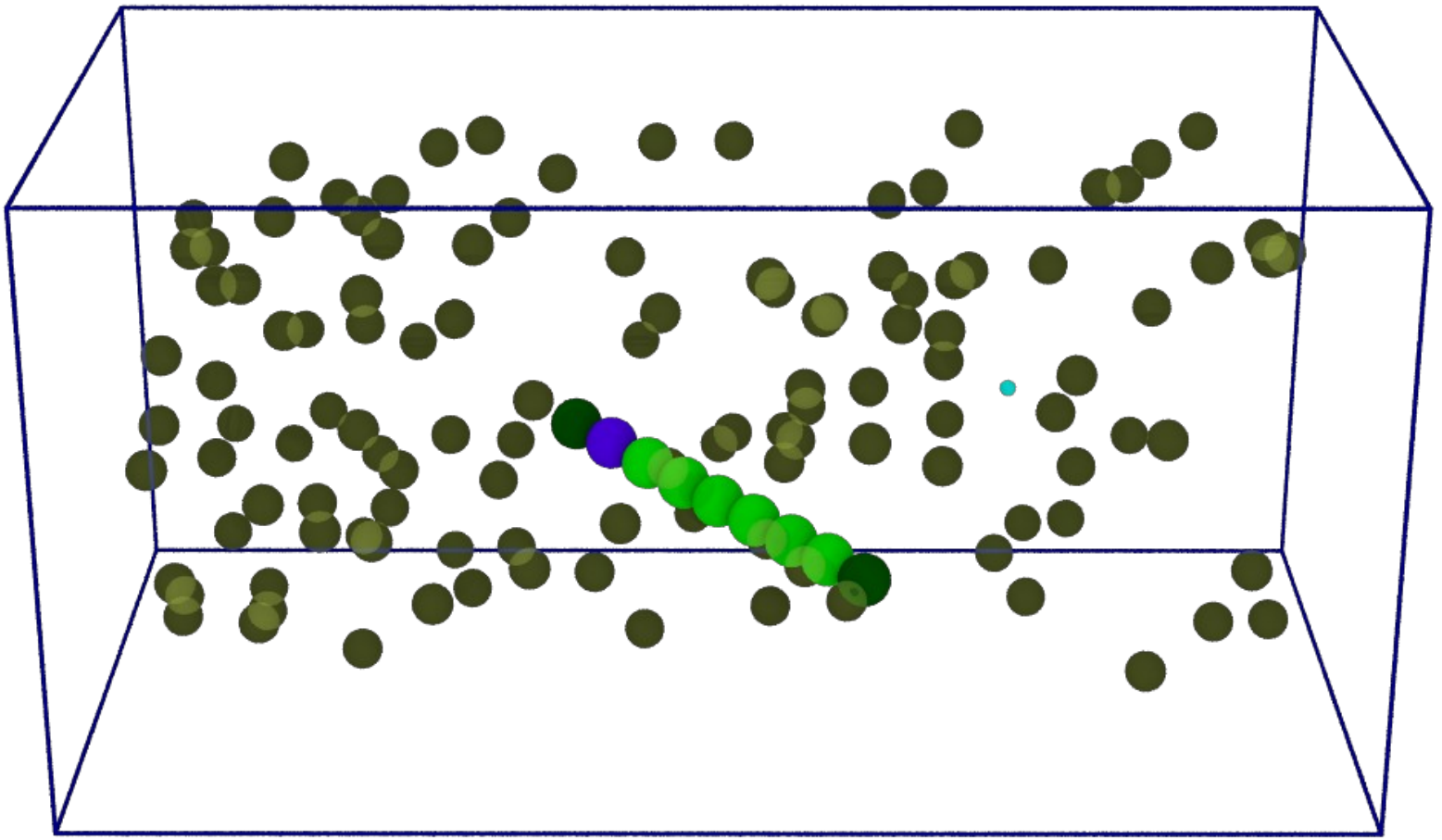

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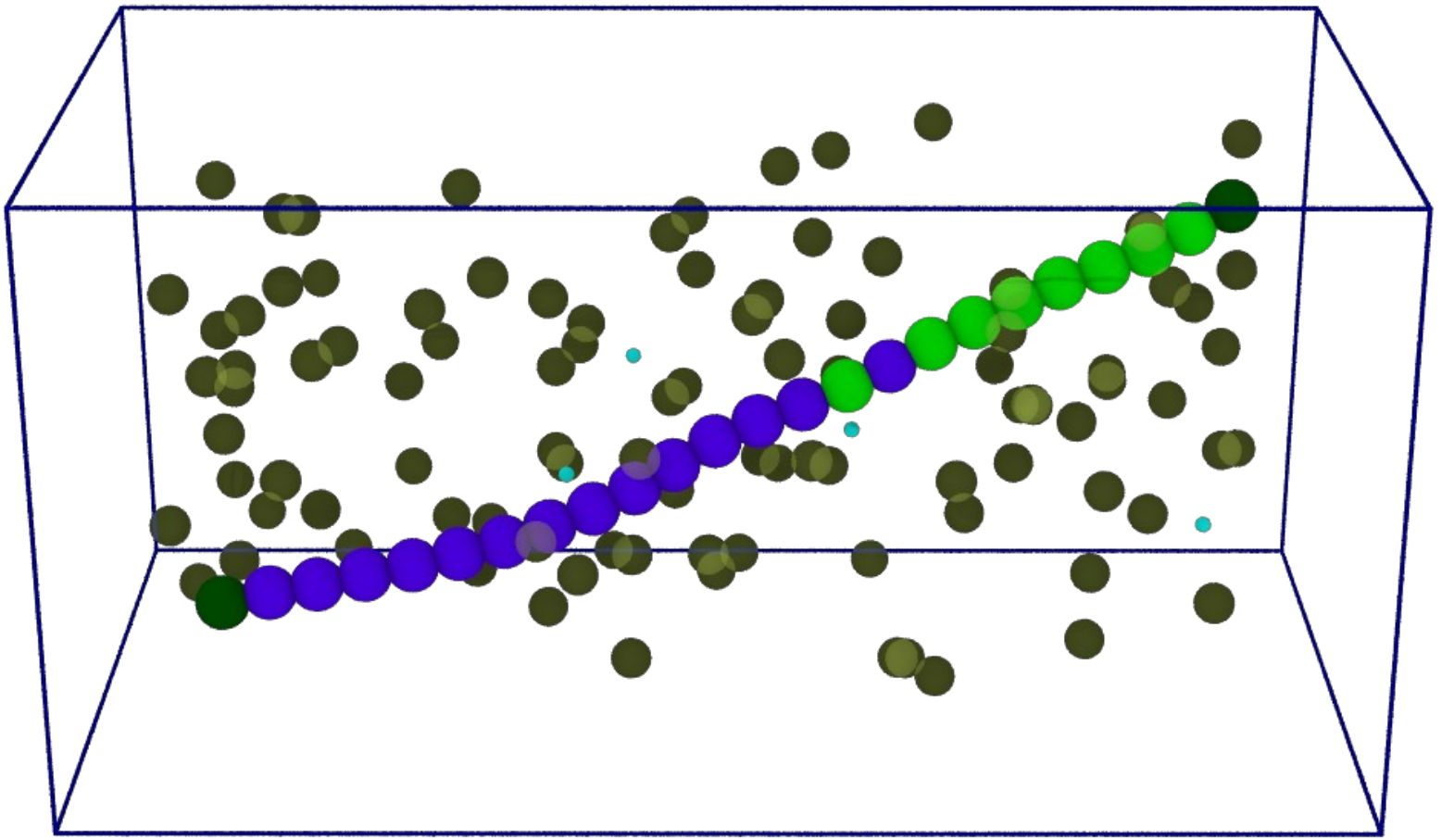

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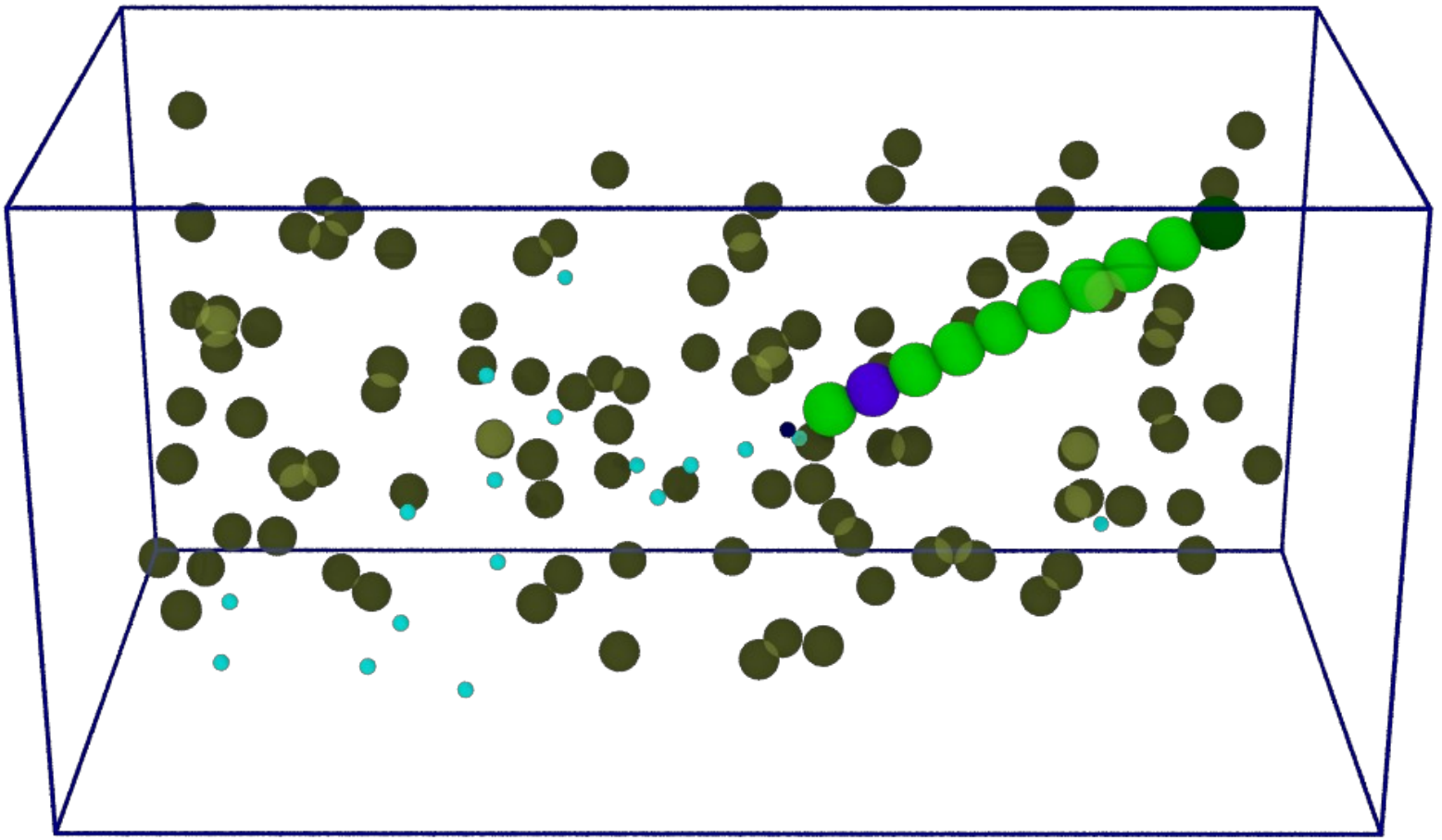

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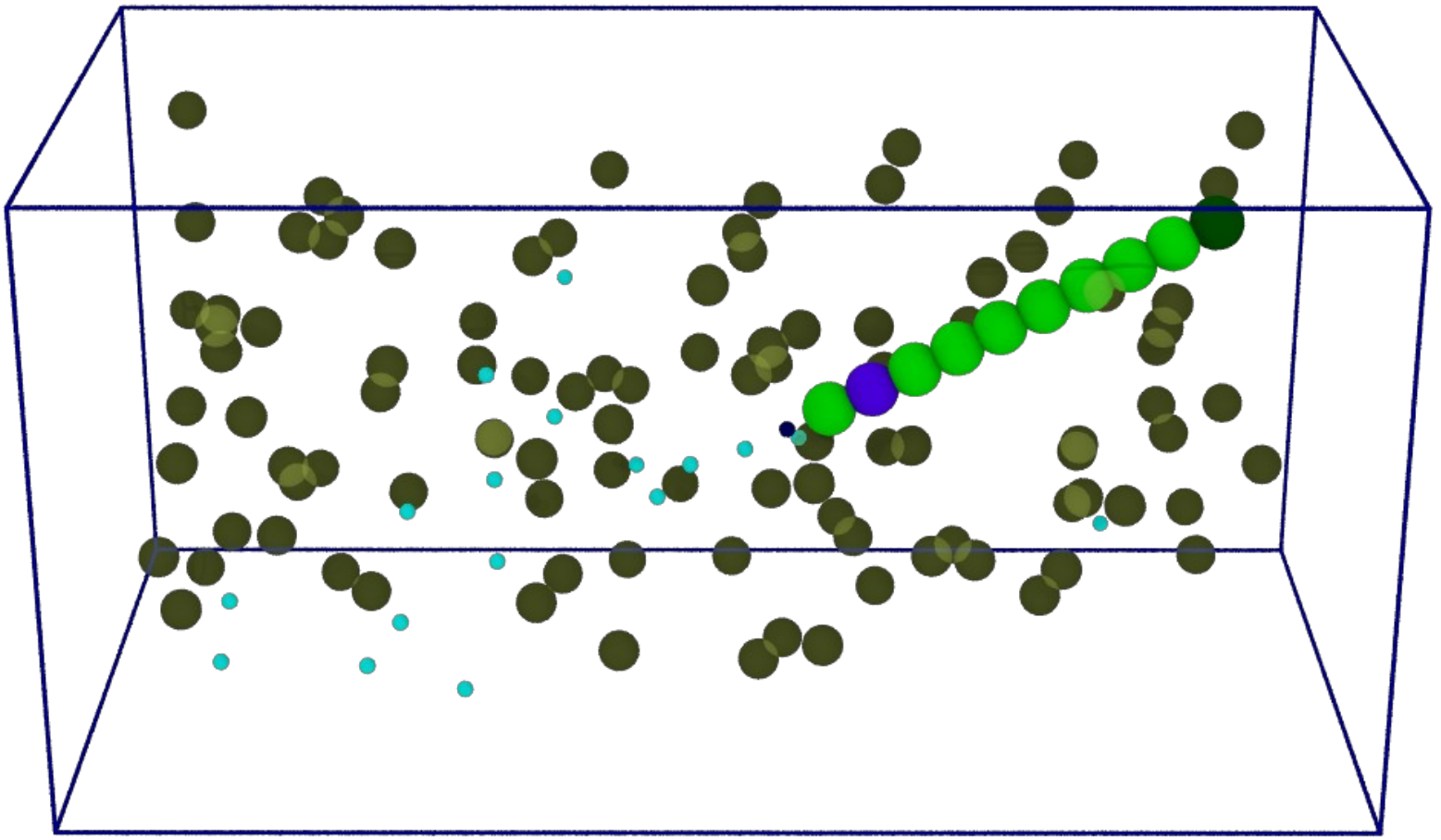
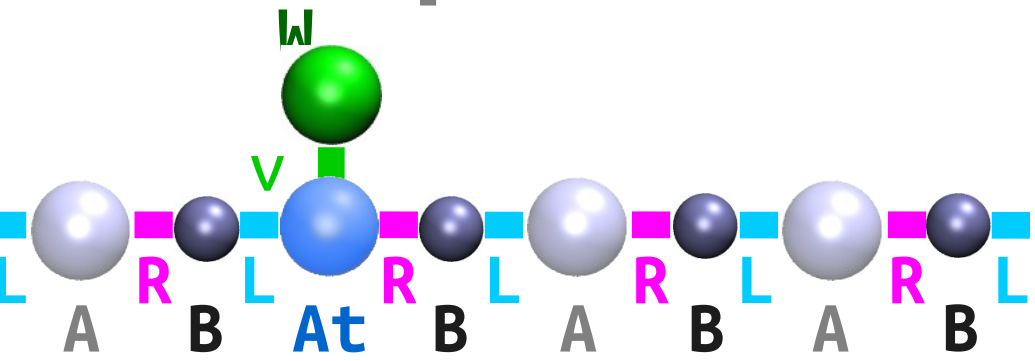
Garner, …, Mullins, Science (2004)

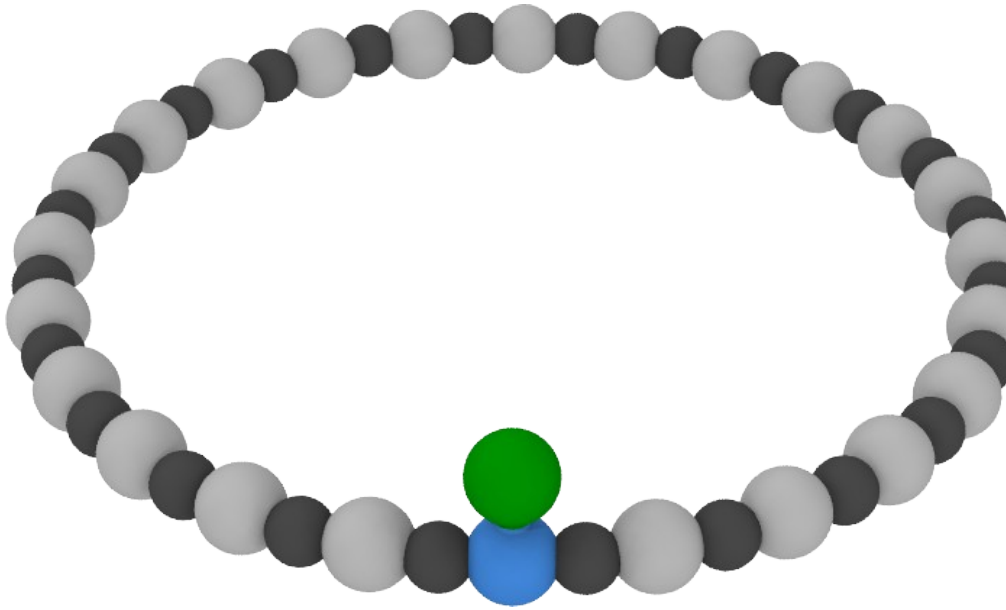
Example 2: Dynamic Instabilty of ParM



SEE:
https://www.youtube.com/watch?v=EEbt07vZHew

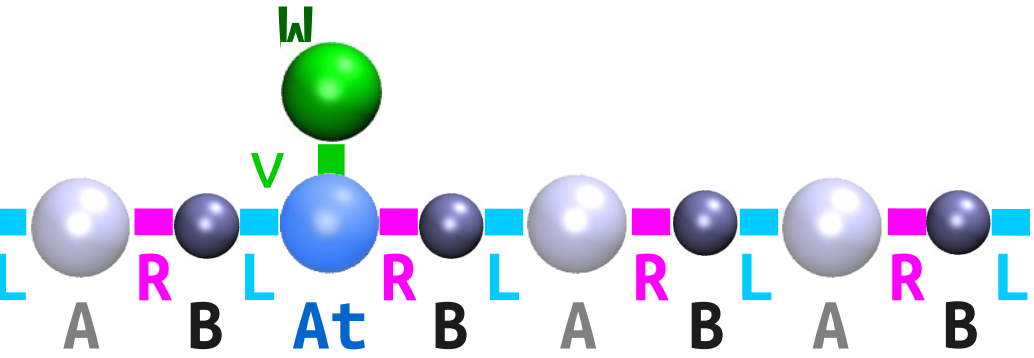
Example: Walking along a polymer

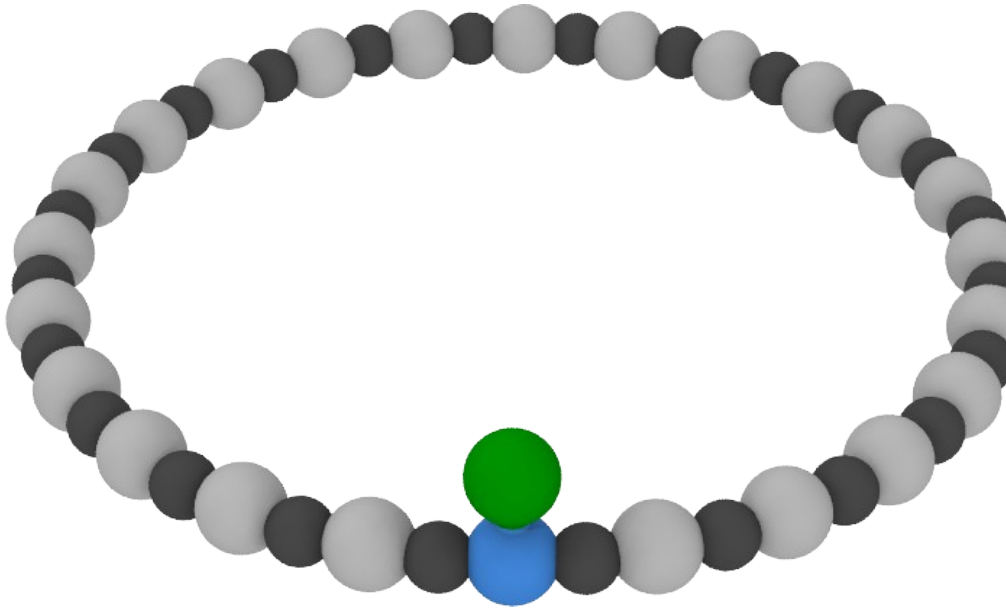




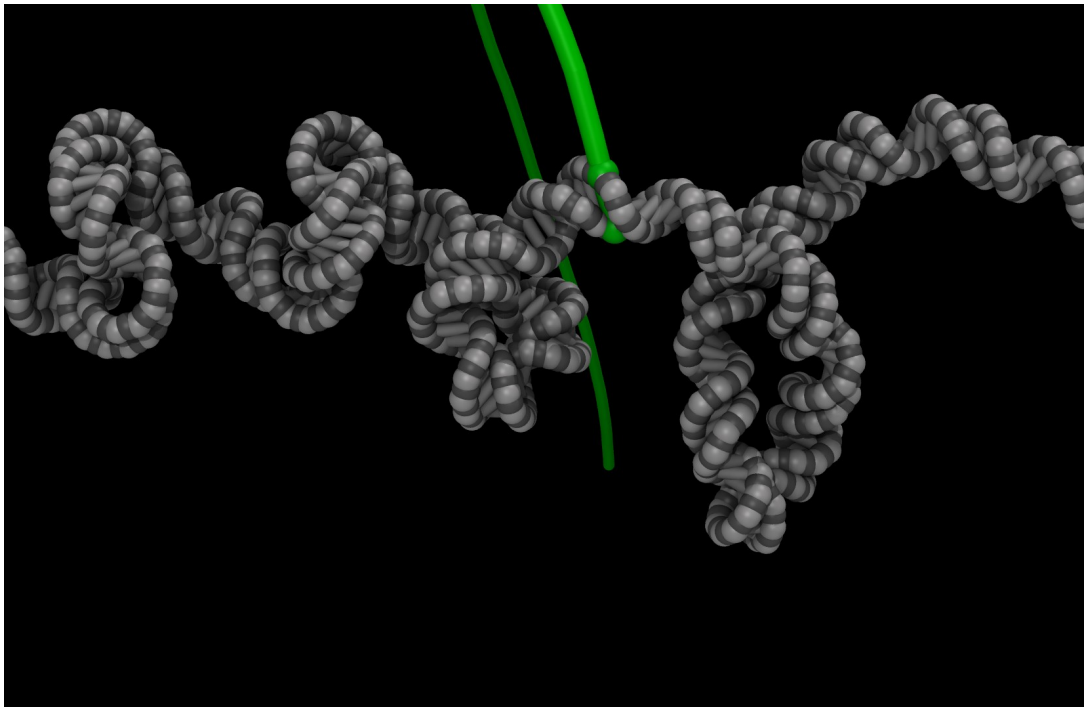
SEE:
https://www.youtube.com/watch?v=QO4LbHGAgxU

Example: DNA supercoiling during transcription

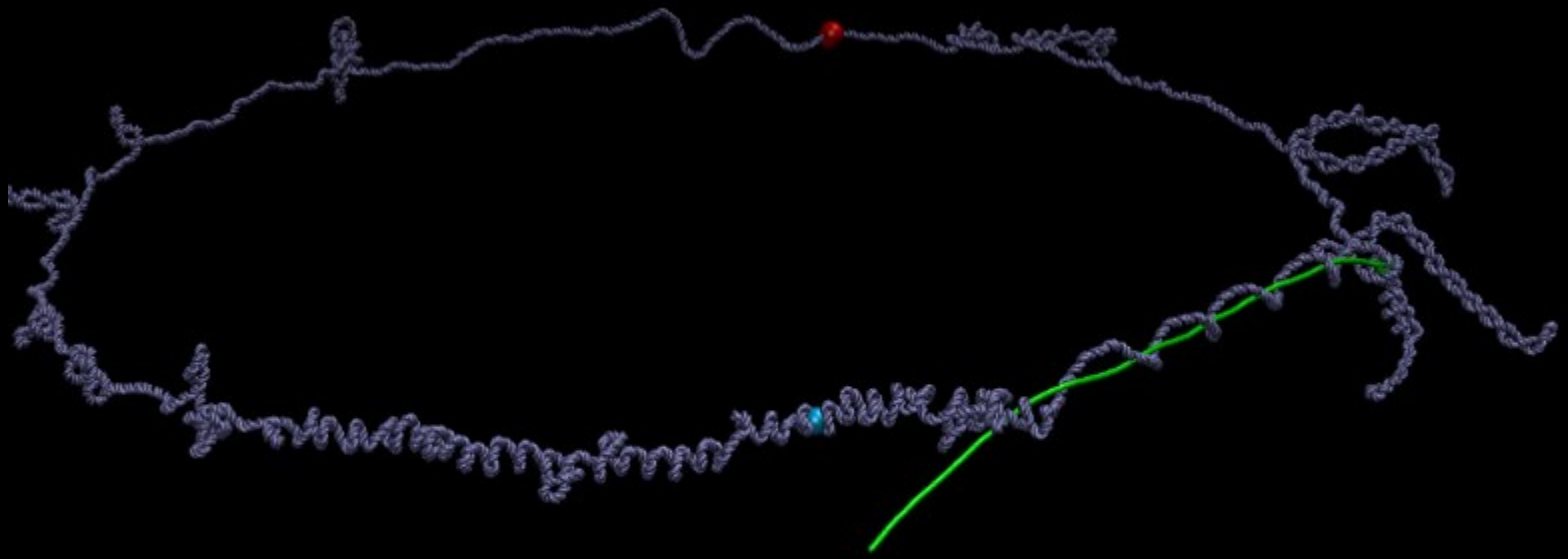




(DNA version with supercoiling)



Example: DNA supercoiling during transcription



Conways Game of Life in Moltemplate

```
 fix ac1 all bond/change 1         &
    atoms @atom:C0  @atom:Live and bond @bond:NeighborUnread
 -> atoms @atom:C1  @atom:Dead and bond @bond:NeighborRead

 fix ac2 all bond/change 1         &
    atoms @atom:C1  @atom:Live and bond @bond:NeighborUnread
 -> atoms @atom:C2  @atom:Dead and bond @bond:NeighborRead

 fix ac3 all bond/change 1         &
    atoms @atom:C2  @atom:Live and bond @bond:NeighborUnread
 -> atoms @atom:C3  @atom:Dead and bond @bond:NeighborRead

 fix ac4 all bond/change 1         &
    atoms @atom:C3  @atom:Live and bond @bond:NeighborUnread
 -> atoms @atom:C4  @atom:Dead and bond @bond:NeighborRead

 fix aResetNeighbors all bond/change 1         &
    bond @bond:NeighborRead  ->  bond @bond:NeighborUnread

 #   Underpopulation: Any live cell with less than 2 living neighbors dies
 fix aUnderpopulation all bond/change 1         &
    atoms @atom:Live @{atom:C0}*@{atom:C1}  and  bond @bond:SendTotal   &
 -> atoms @atom:Dead SAME

#   Overpopulation:  Any live cell with 4 living neighbors dies
 fix aOverpopulation all bond/change 1         &
    atoms @atom:Live @atom:C4  and  bond @bond:SendTotal   &
 -> atoms @atom:Dead SAME

 #   Birth:           Any dead cell with exactly 3 living neighbors lives
 fix aBirth all bond/change 1         &
    atoms @atom:Dead @atom:C3 and  bond @bond:SendTotal   &
 -> atoms @atom:Live SAME

 fix aResetCounters all atom/change 1         &
    atom *  ->  atom @atom:C0
```