Example: Walking along a polymer

We want the green bead to "walk" along the polymer
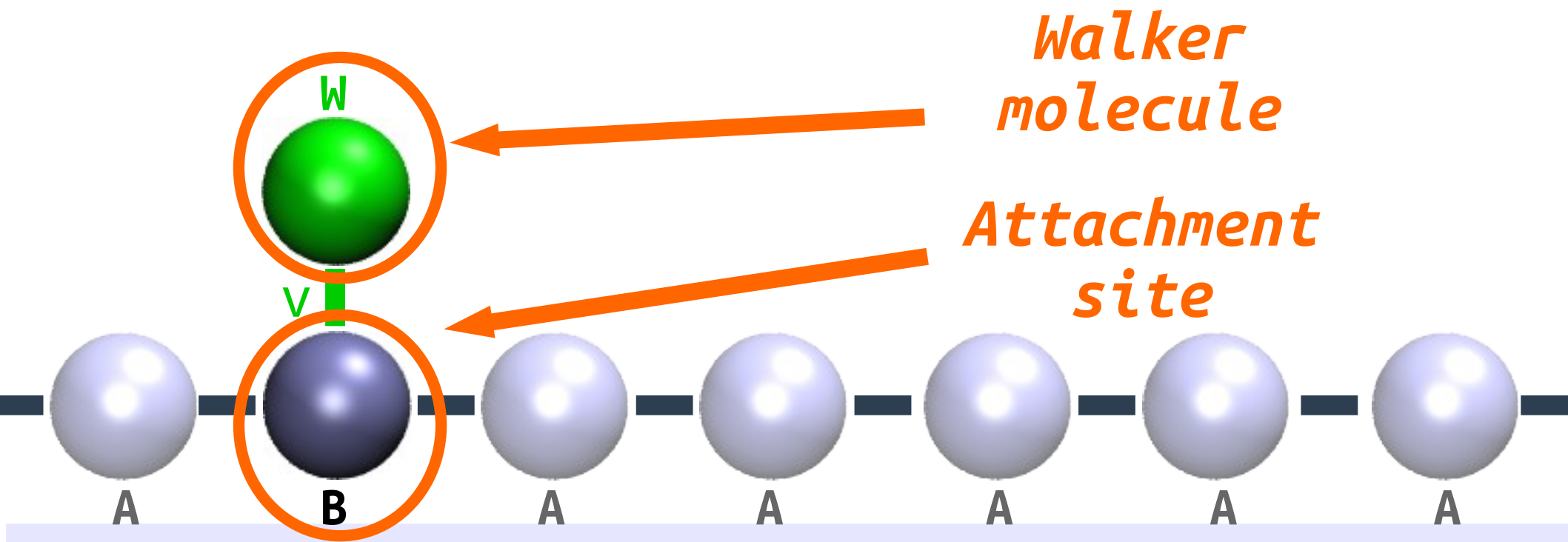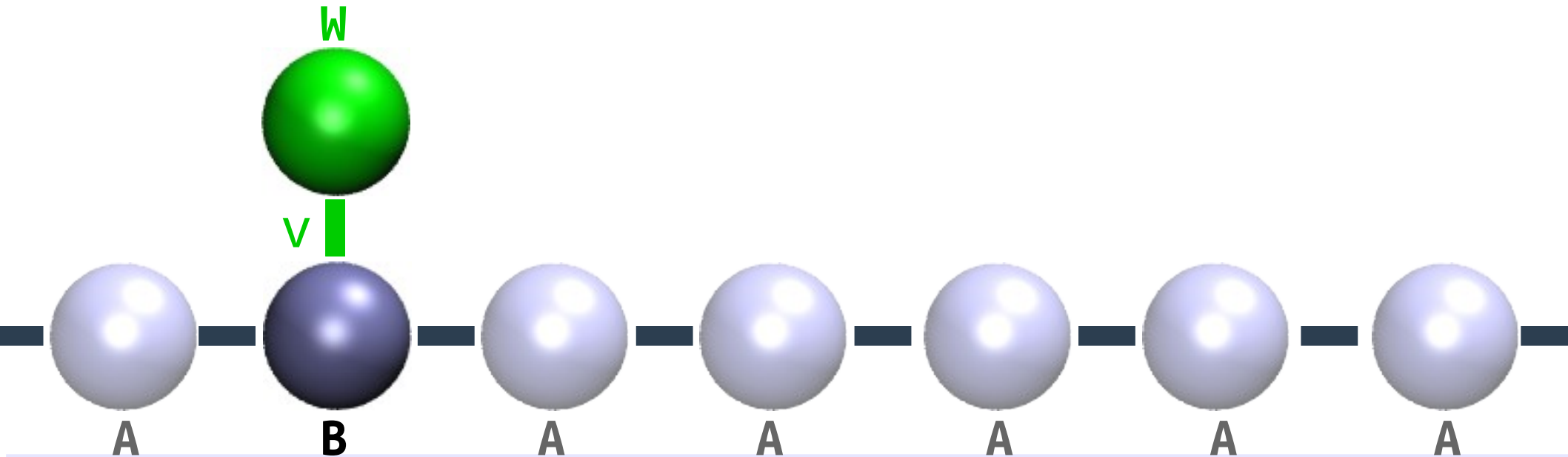
Walker
molecule

Attachment
site

W

v

A B A A A A A

Example: Walking along a polymer
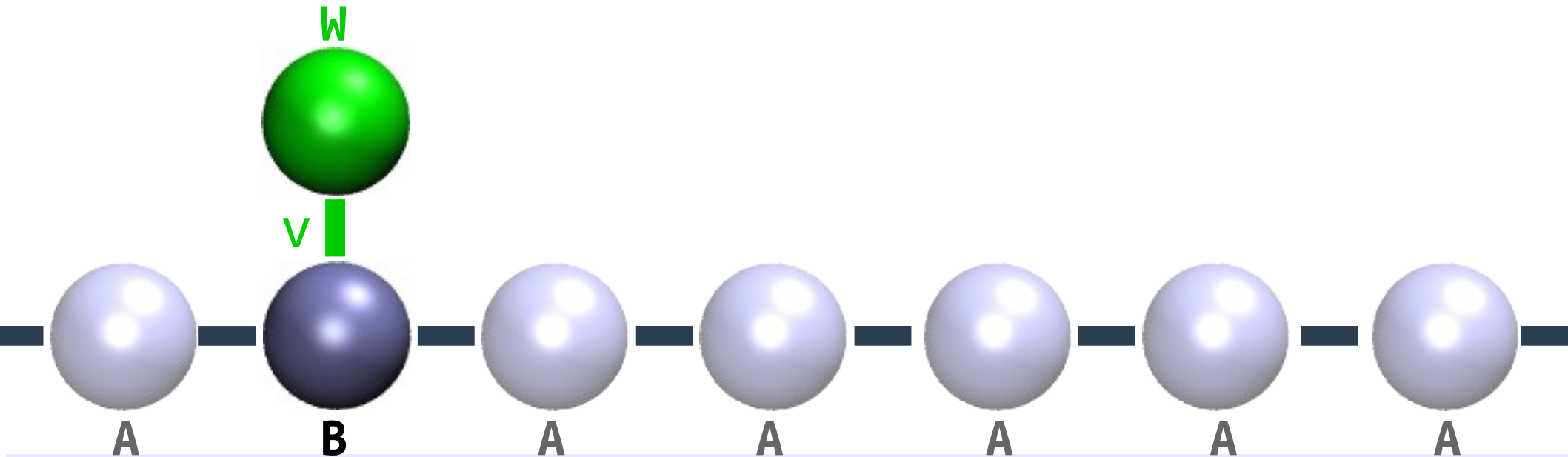


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
  if atoms @atom:Wt @atom:A
  -> atoms @atom:W  @atom:A  and  bond BREAK
```
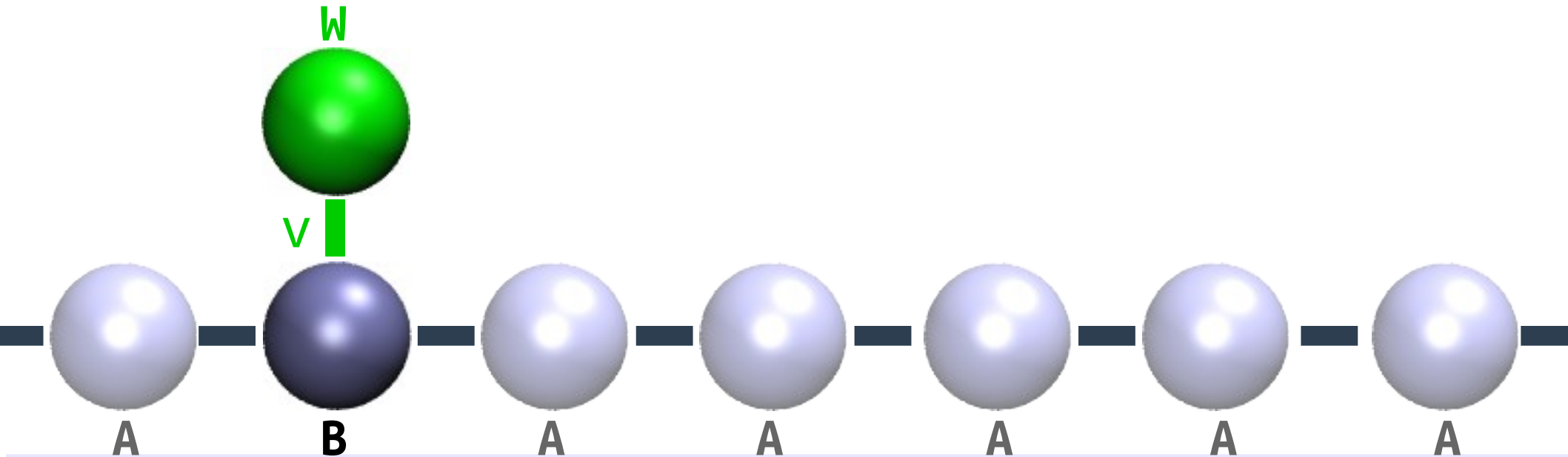
Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt
```

Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt
```

Example: Walking along a polymer
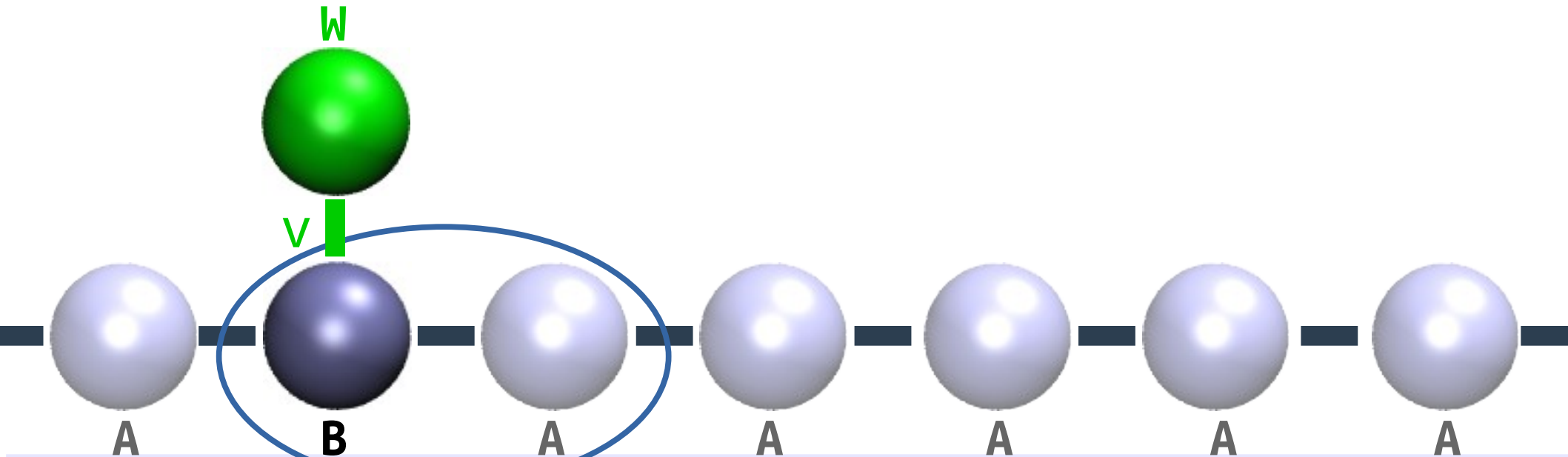


```
fix tr1  all bond/change 100  delay 1
   if atoms @atom:B  @atom:A  and  ordered
   -> atoms @atom:A  @atom:Bt
```

Example: Walking along a polymer
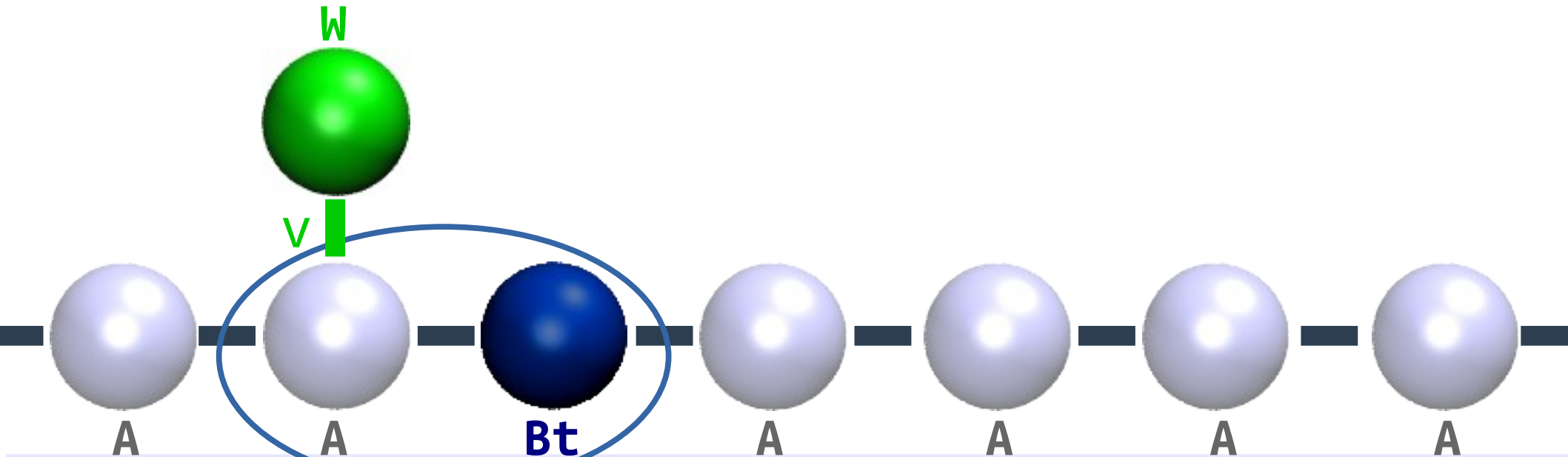


```
fix tr1  all bond/change 100  delay 1
   if atoms @atom:B  @atom:A   and  ordered
   -> atoms @atom:A  @atom:Bt
```

Example: Walking along a polymer
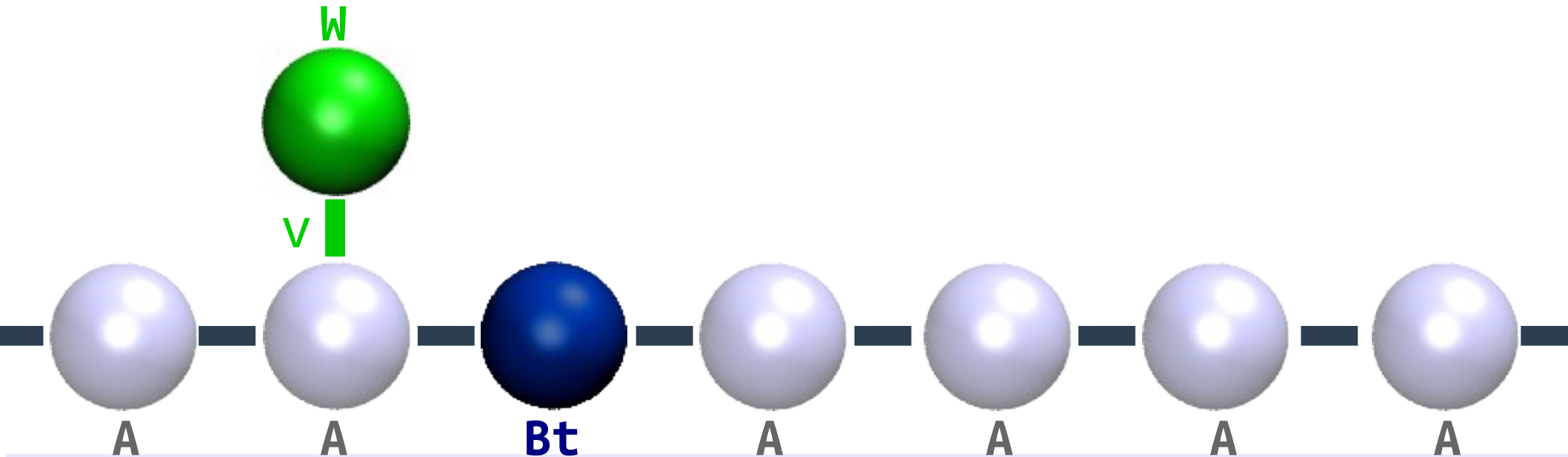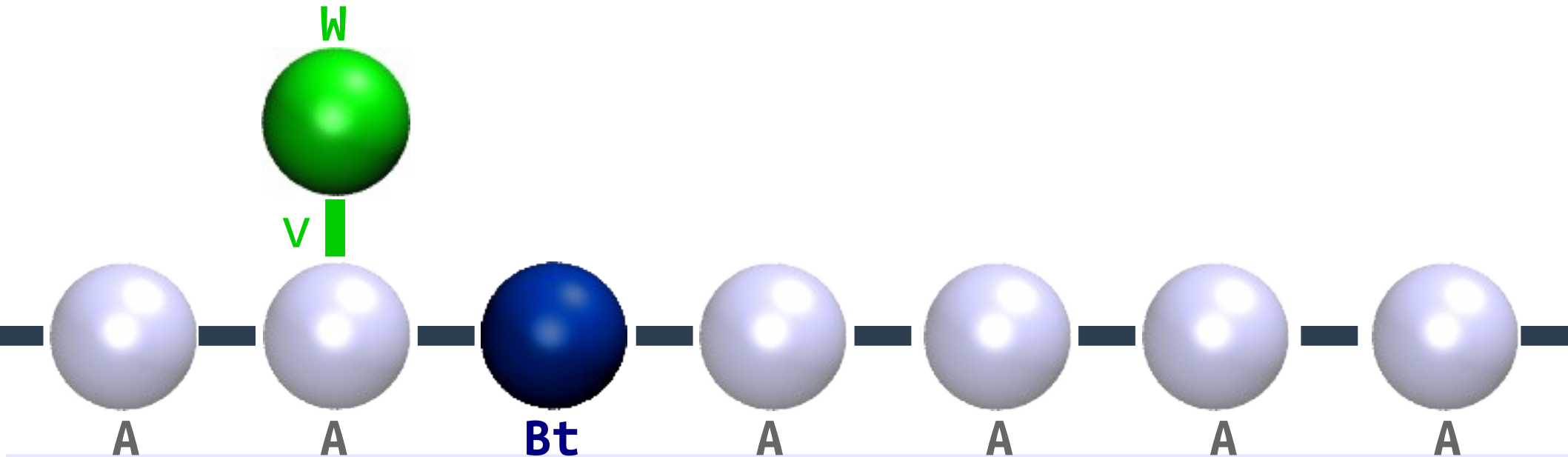


```
fix tr1   all bond/change 100   delay 1
   if atoms @atom:B  @atom:A  and  ordered
   -> atoms @atom:A  @atom:Bt
```

Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
   if atoms @atom:B  @atom:A  and  ordered
   -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
   if atoms @atom:W  @atom:Bt and  distance <= 1.5
   -> atoms @atom:Wt @atom:B  and  bond @bond:V
```

Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new   100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V
```

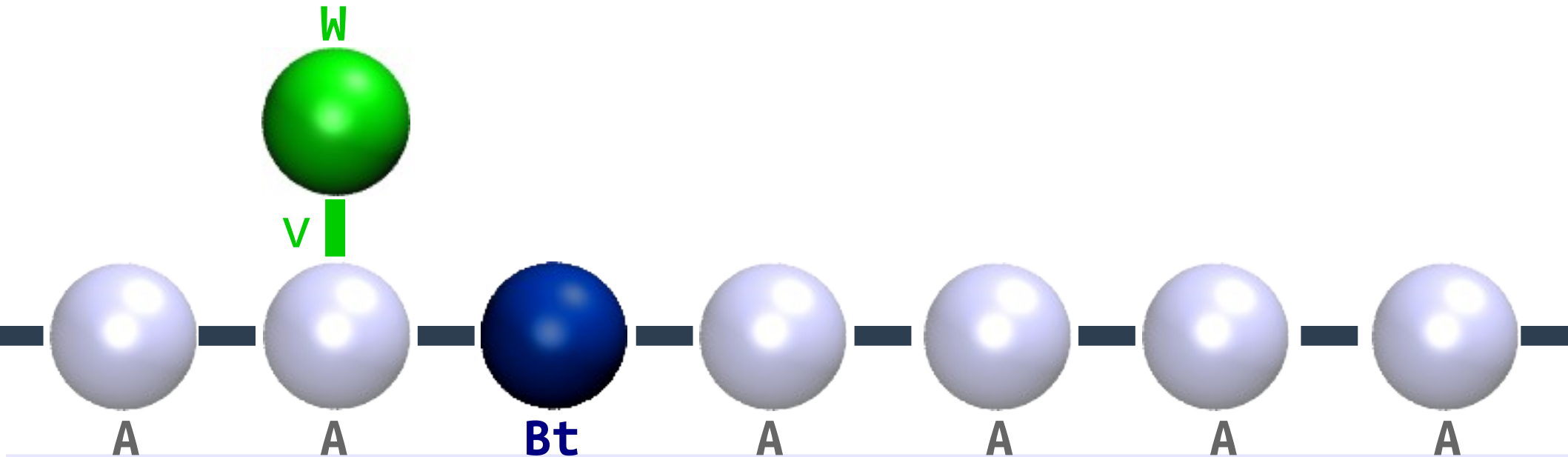# Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V
```
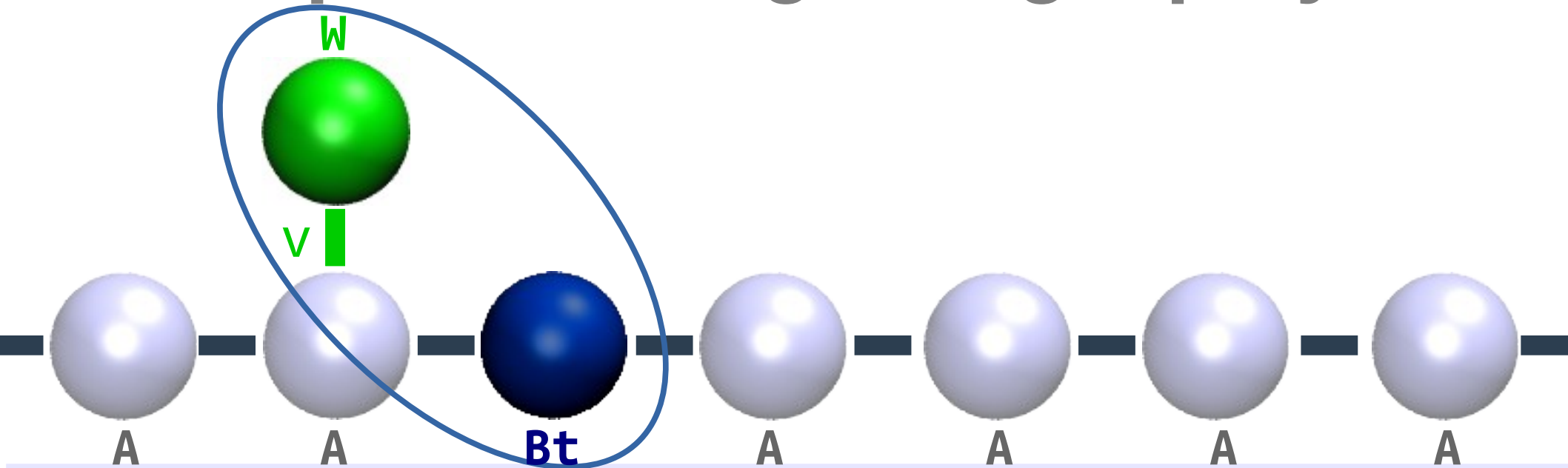
Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
   if atoms @atom:B  @atom:A  and  ordered
   -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new     100  delay 2
   if atoms @atom:W  @atom:Bt and  distance <= 1.5
   -> atoms @atom:Wt @atom:B  and  bond @bond:V
```
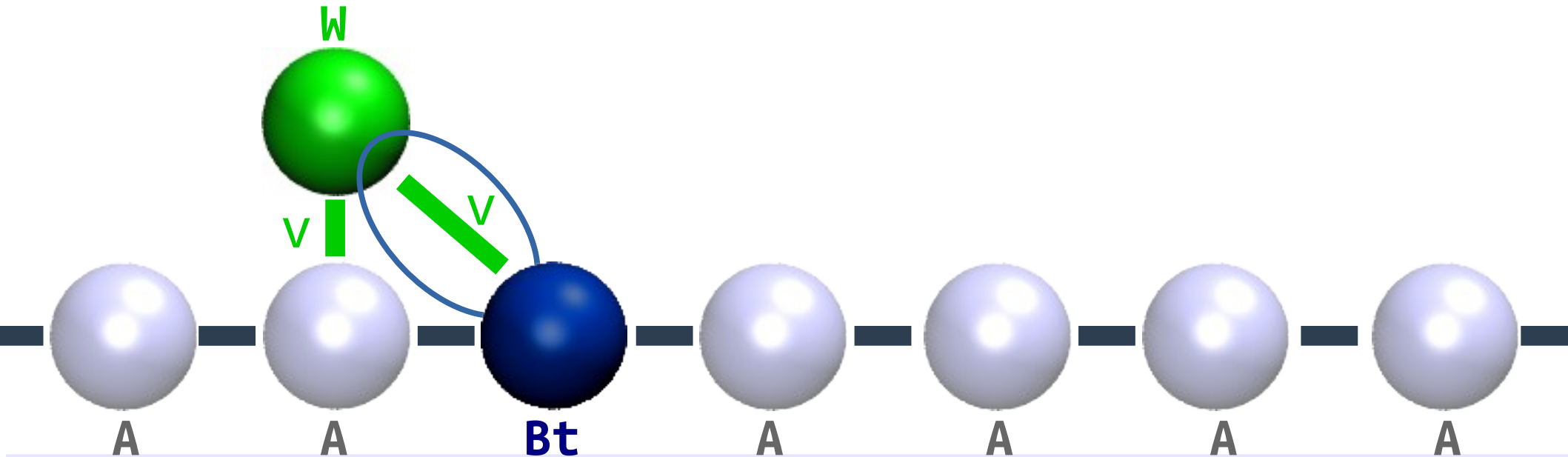
Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V
```

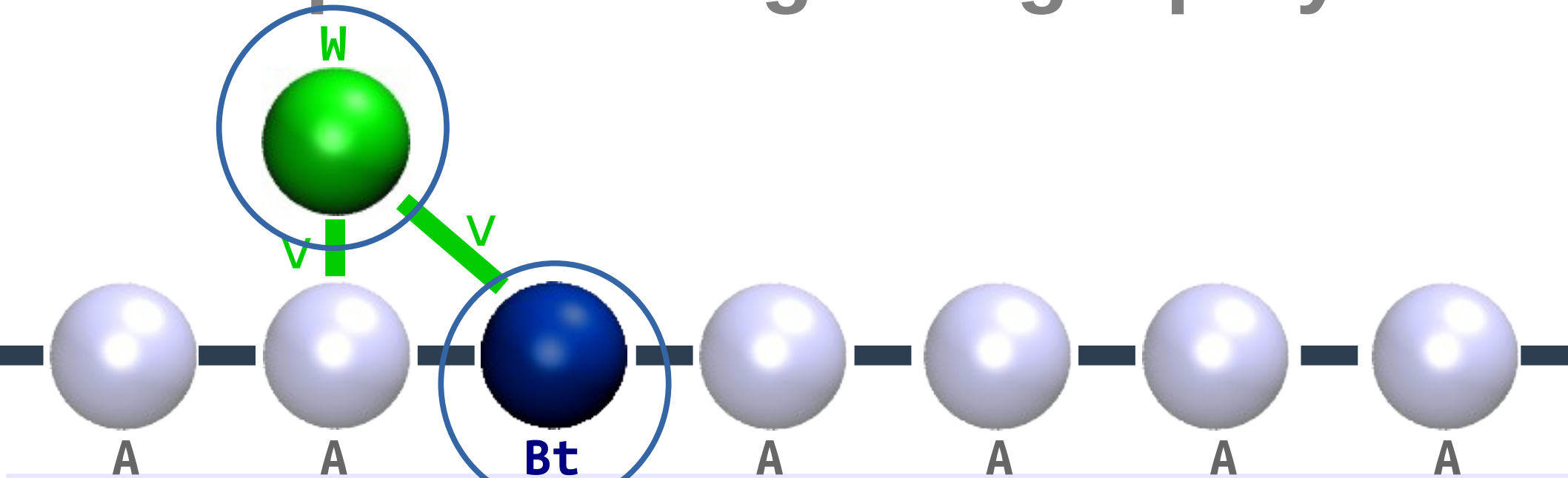# Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V
```

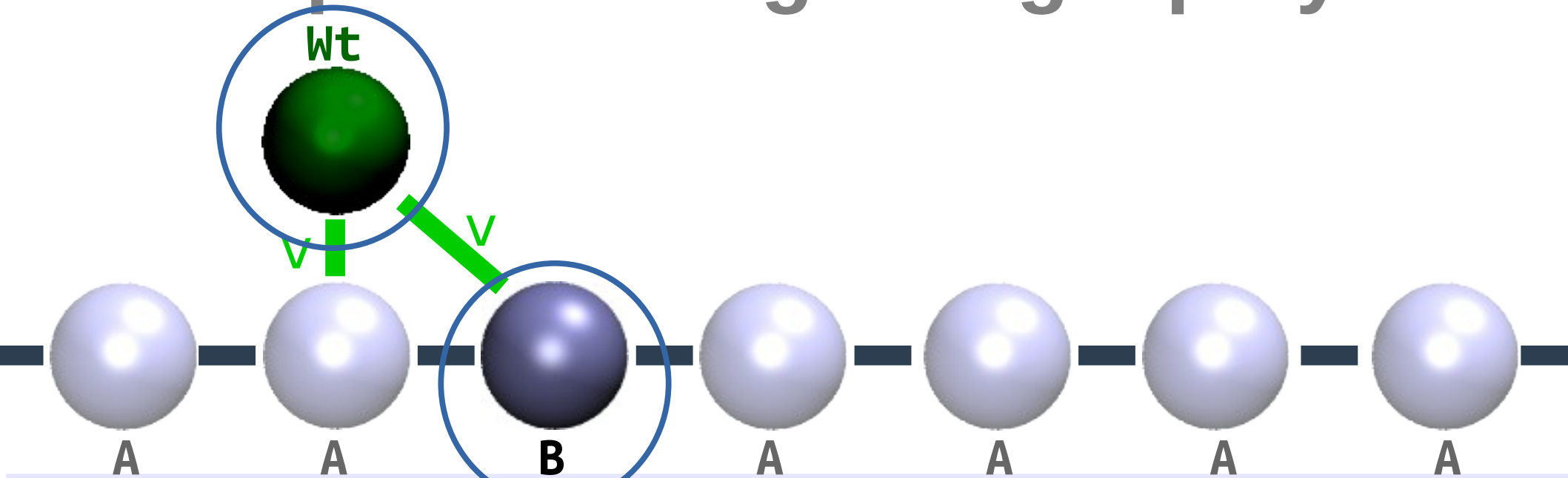# Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new     100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V
```

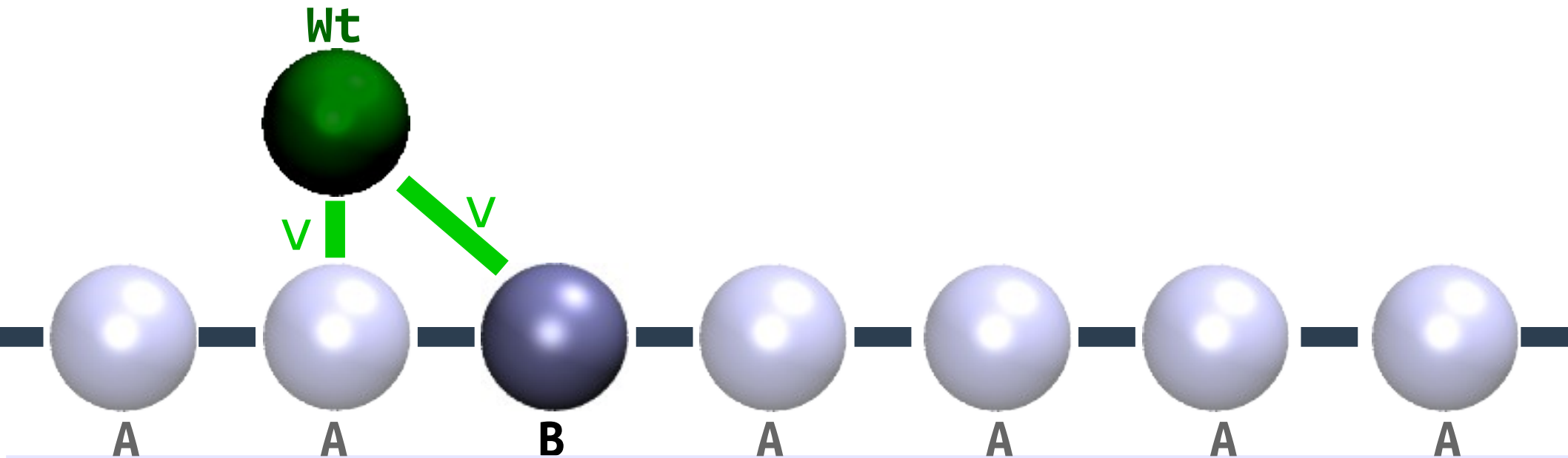# Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
  if atoms @atom:Wt @atom:A
  -> atoms @atom:W  @atom:A  and  bond BREAK
```
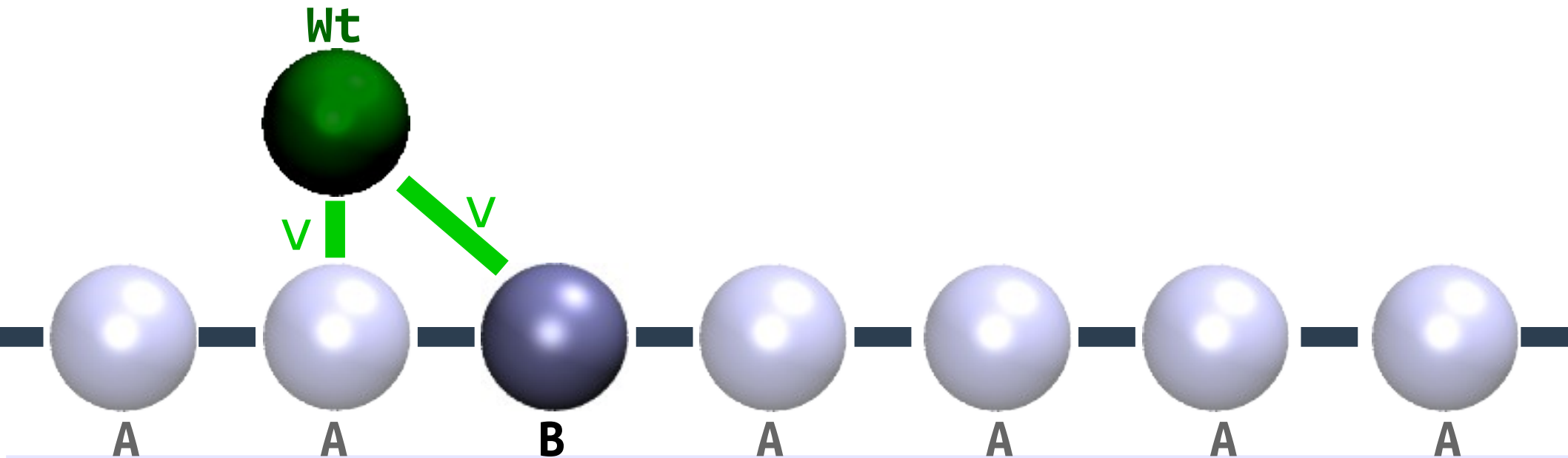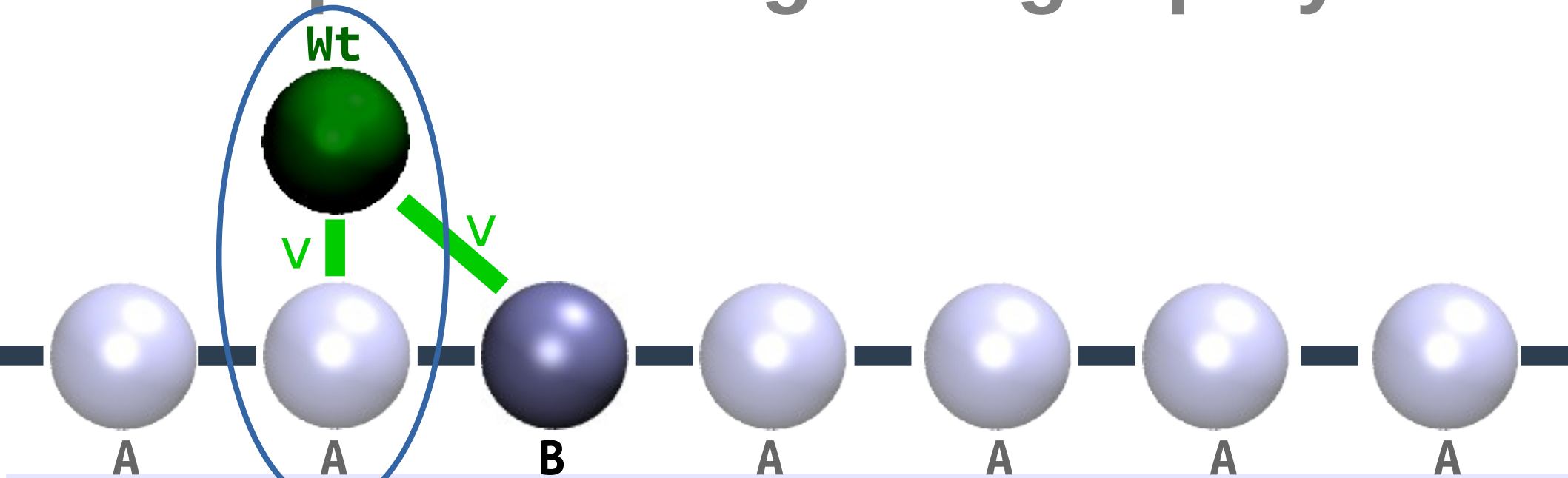
Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
  if atoms @atom:Wt @atom:A
  -> atoms @atom:W  @atom:A  and  bond BREAK
```
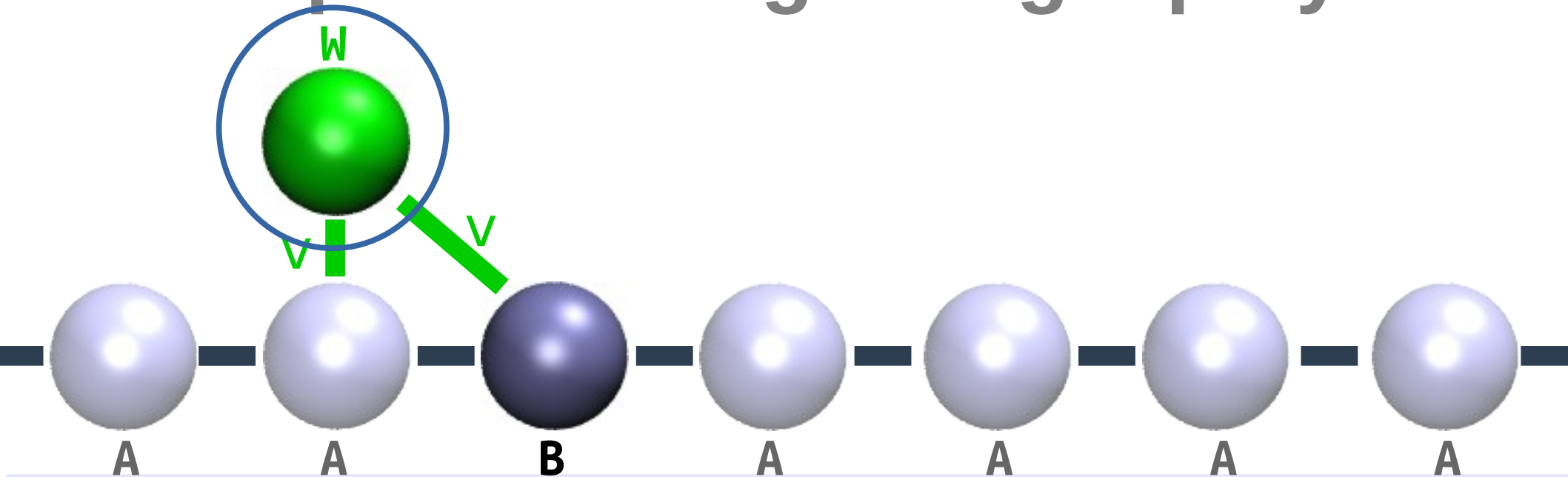
Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
  if atoms @atom:Wt @atom:A
  -> atoms @atom:W  @atom:A  and  bond BREAK
```
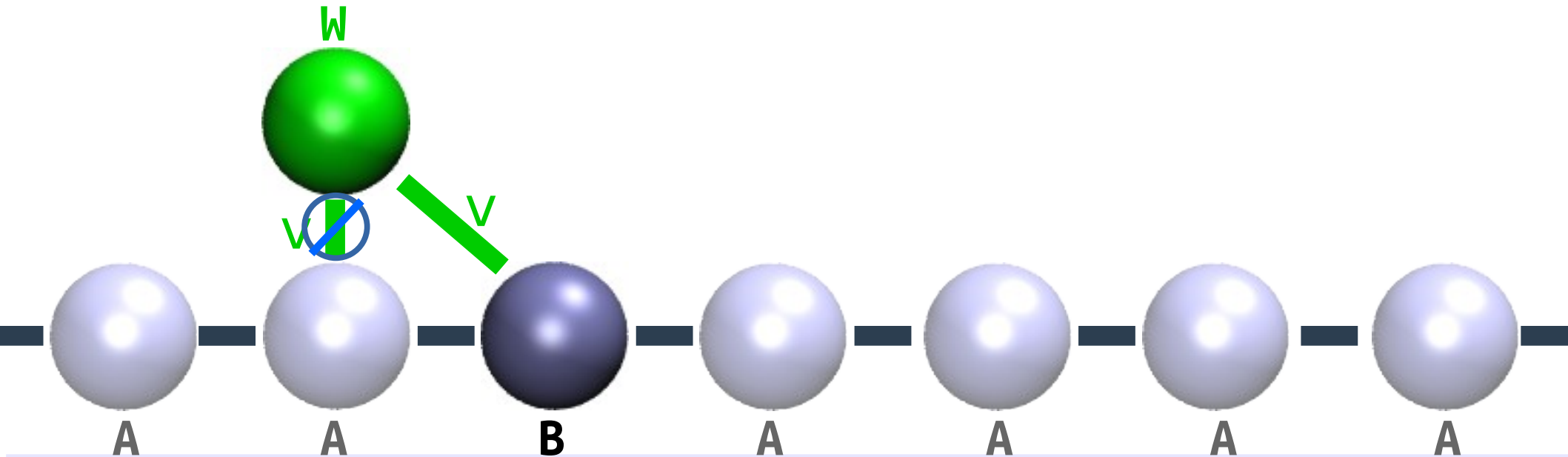
Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
  if atoms @atom:Wt @atom:A
  -> atoms @atom:W  @atom:A  and  bond BREAK
```
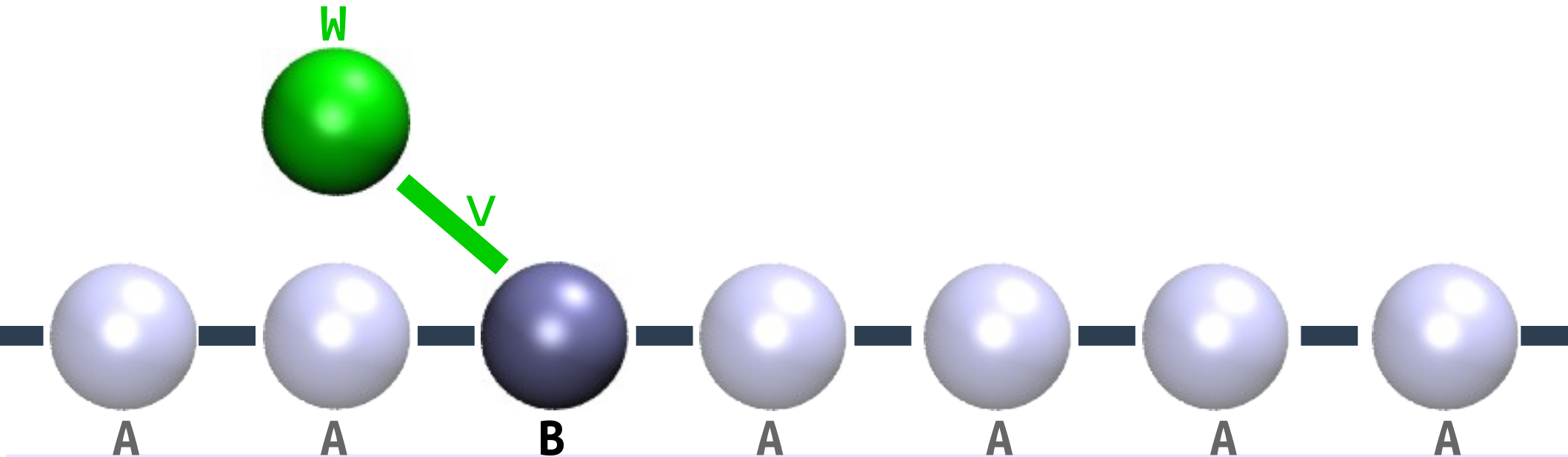
Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
  if atoms @atom:Wt @atom:A
  -> atoms @atom:W  @atom:A  and  bond BREAK
```
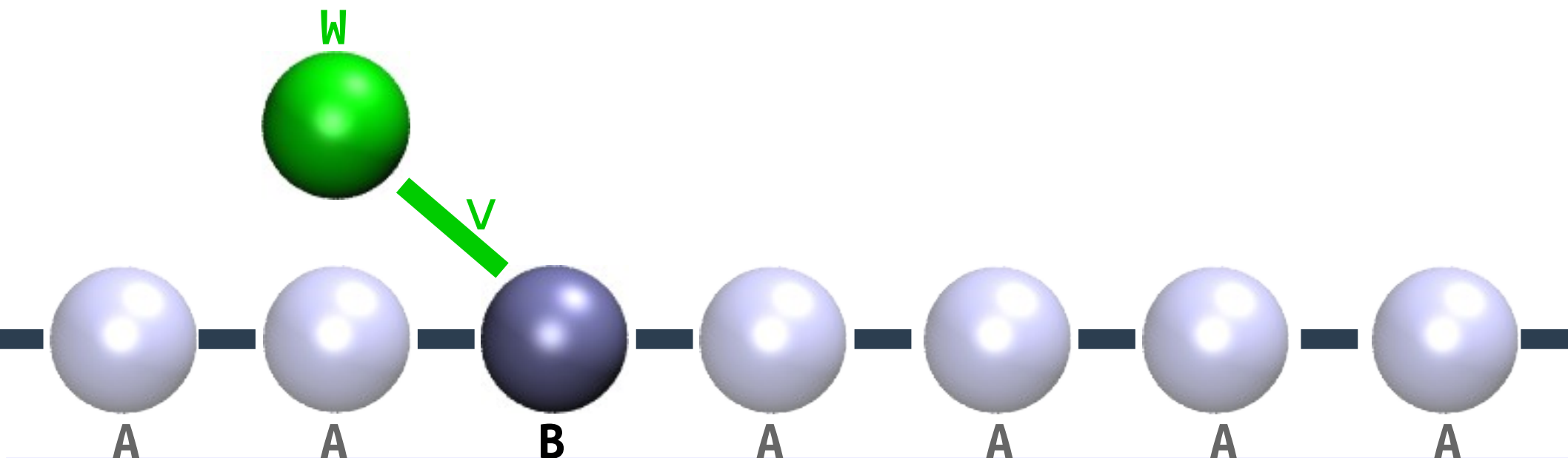
Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
  if atoms @atom:Wt @atom:A
  -> atoms @atom:W  @atom:A  and  bond BREAK
```
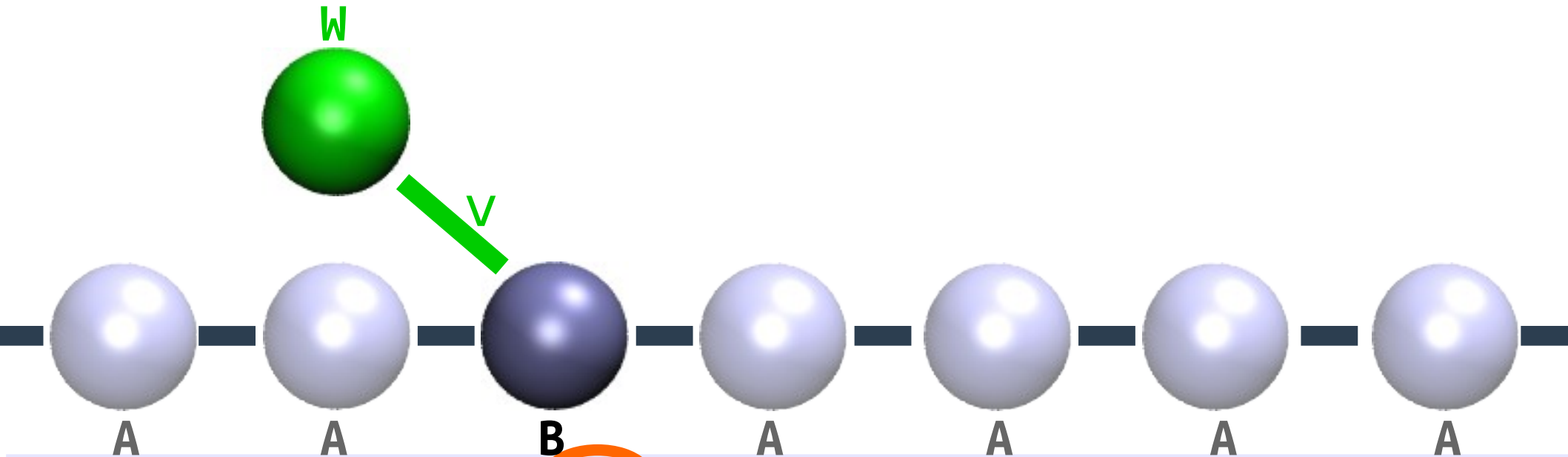
Example: Walking along a polymer


```
fix tr1  all bond/change  100  delay 1
   if atoms @atom:B  @atom:A  and  ordered
   -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new     100  delay 2
   if atoms @atom:W  @atom:Bt and  distance <= 1.5
   -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify  100  delay 3
   if atoms @atom:Wt @atom:A
   -> atoms @atom:W  @atom:A  and  bond BREAK
```

NOW RUN MOLECULAR DYNAMICS

(allow particles to move)

Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
    if atoms @atom:B  @atom:A  and  ordered
    -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new     100  delay 2
    if atoms @atom:W  @atom:Bt and  distance <= 1.5
    -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
    if atoms @atom:Wt @atom:A
    -> atoms @atom:W  @atom:A  and  bond BREAK
```
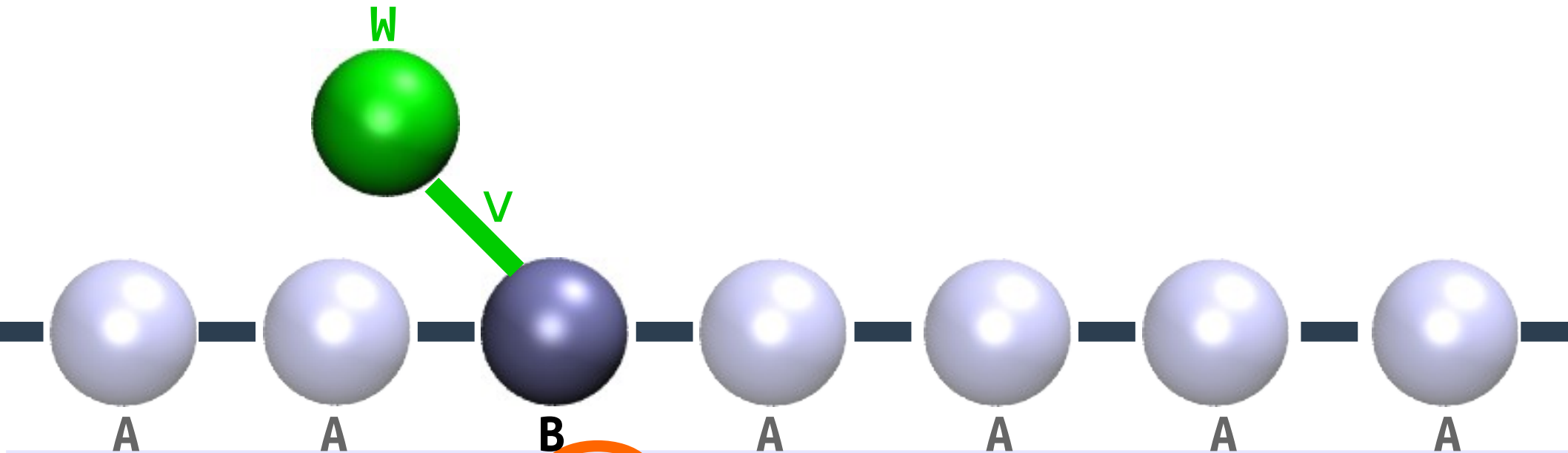
NOW RUN MOLECULAR DYNAMICS

(allow particles to move)

Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
   if atoms @atom:B  @atom:A  and  ordered
   -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new     100  delay 2
   if atoms @atom:W  @atom:Bt and  distance <= 1.5
   -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
   if atoms @atom:Wt @atom:A
   -> atoms @atom:W  @atom:A  and  bond BREAK
```
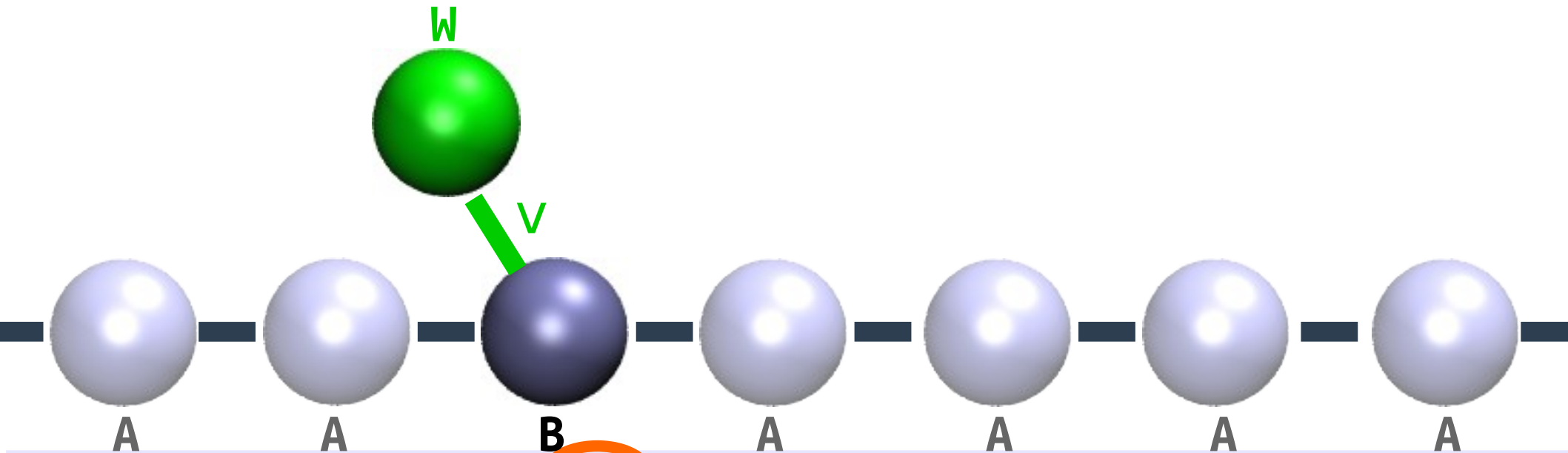
NOW RUN MOLECULAR DYNAMICS

(allow particles to move)

Example: Walking along a polymer


```
fix tr1  all bond/change  100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new     100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:v

fix tr3  all bond/modify  100  delay 3
  if atoms @atom:Wt @atom:A
  -> atoms @atom:W  @atom:A  and  bond BREAK
```
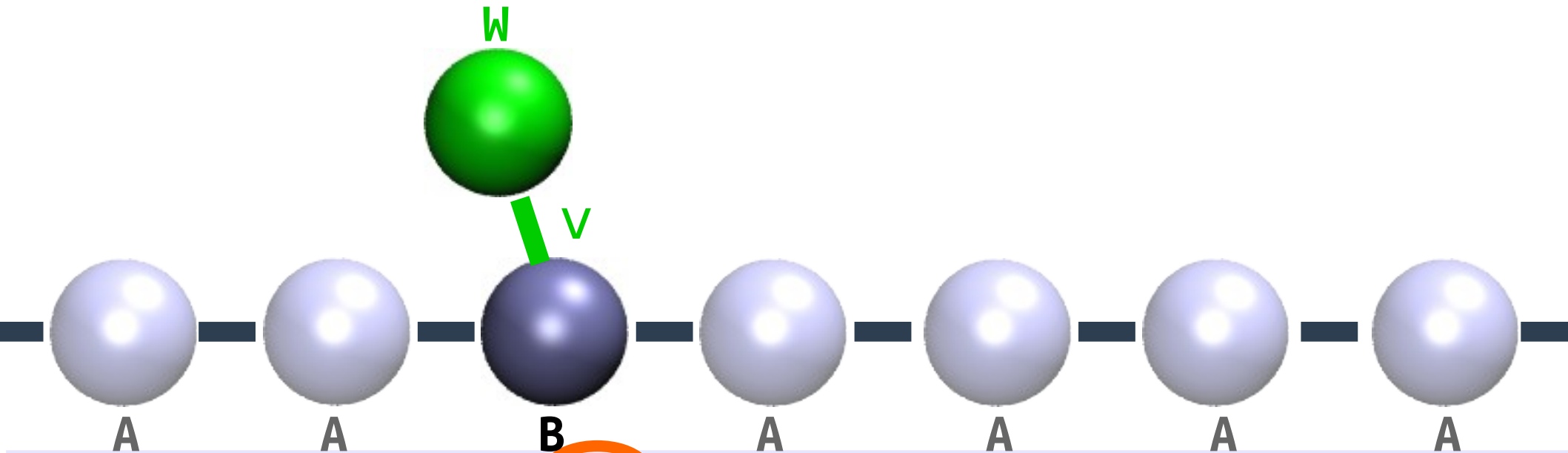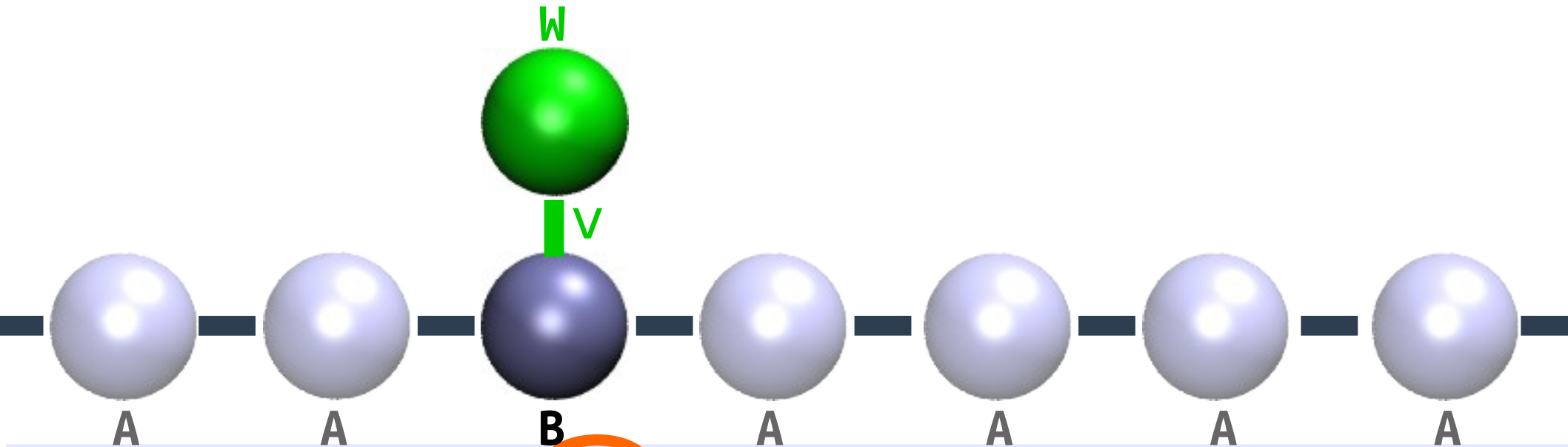
NOW RUN MOLECULAR DYNAMICS

(allow particles to move)

Example: Walking along a polymer


```
fix tr1  all bond/change 100  delay 1
   if atoms @atom:B  @atom:A   and   ordered
   -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
   if atoms @atom:W  @atom:Bt and   distance <= 1.5
   -> atoms @atom:Wt @atom:B  and   bond @bond:V

fix tr3  all bond/modify 100  delay 3
   if atoms @atom:Wt @atom:A
   -> atoms @atom:W  @atom:A  and   bond BREAK
```
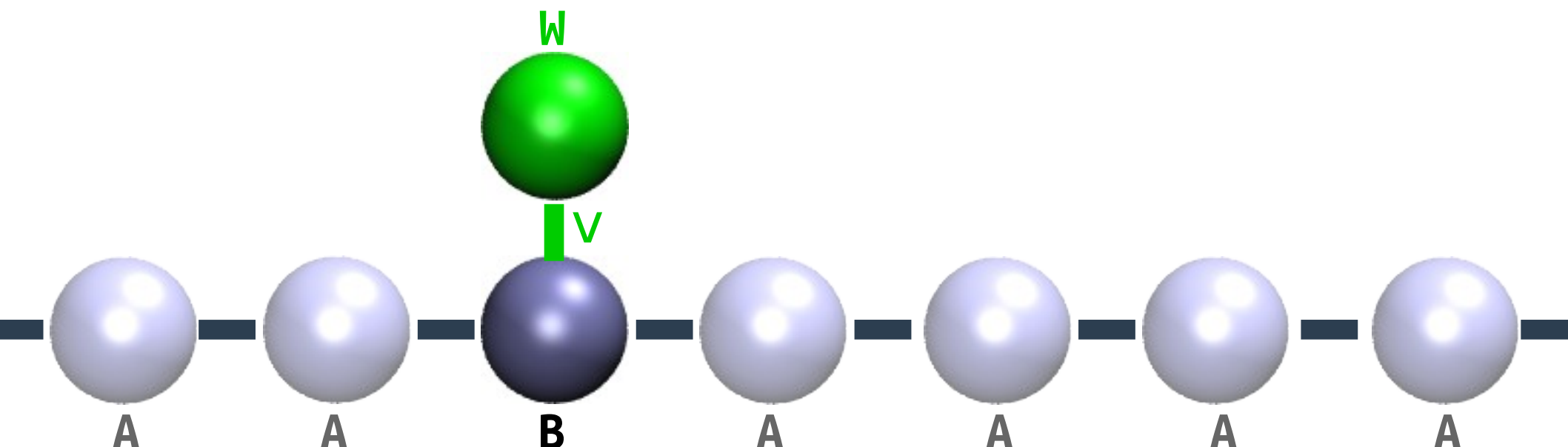
NOW RUN MOLECULAR DYNAMICS

(allow particles to move)

Example: Walking along a polymer
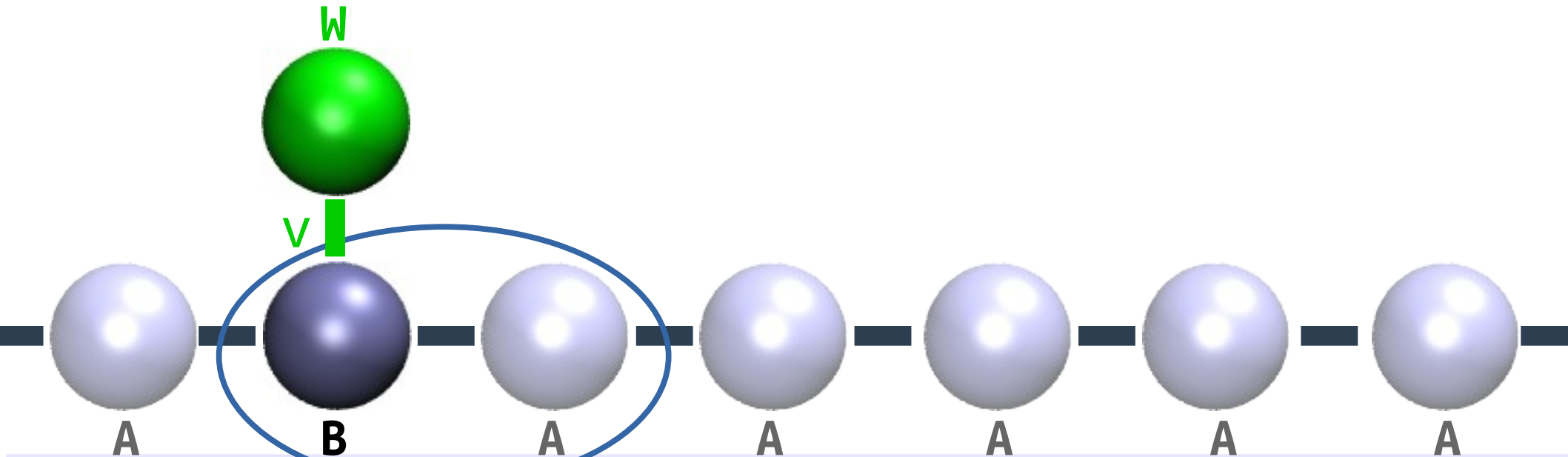


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt

fix tr2  all bond/new    100  delay 2
  if atoms @atom:W  @atom:Bt and  distance <= 1.5
  -> atoms @atom:Wt @atom:B  and  bond @bond:V

fix tr3  all bond/modify 100  delay 3
  if atoms @atom:Wt @atom:A
  -> atoms @atom:W  @atom:A  and  bond BREAK
```
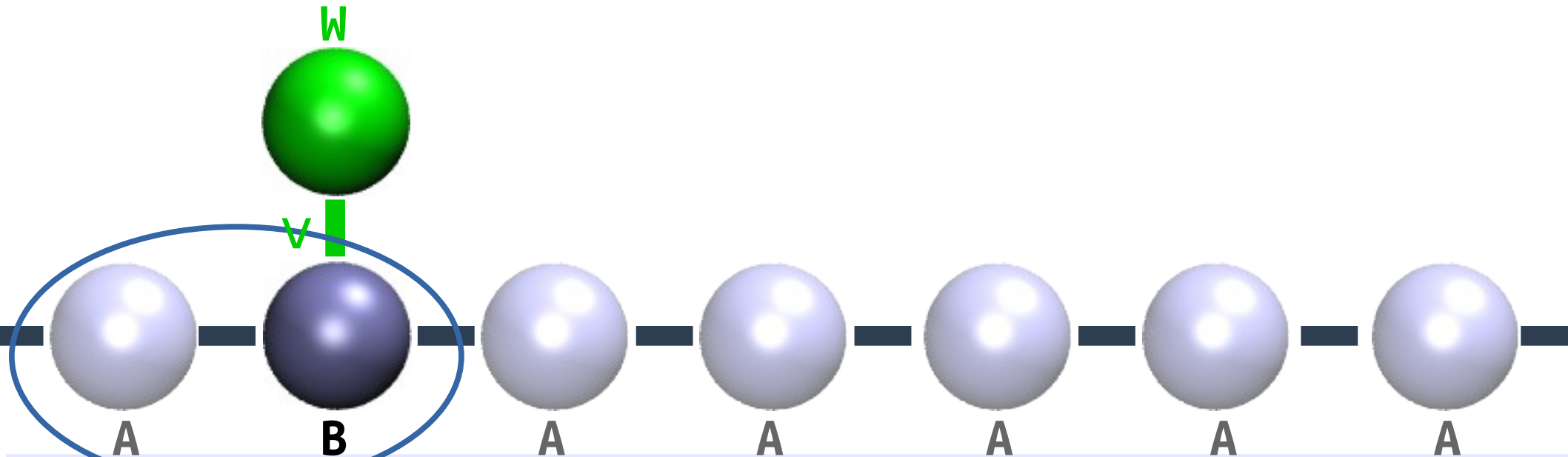
Problem: direction ambiguity

```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt
```

"Walker" can move right or left...
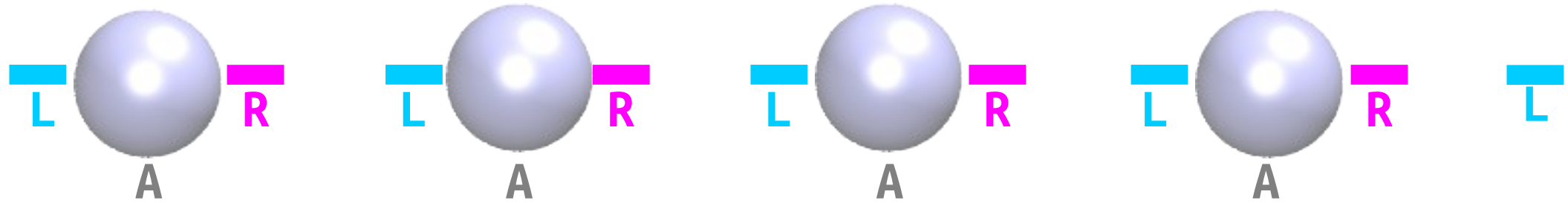
Problem: direction ambiguity


```
fix tr1  all bond/change 100  delay 1
  if atoms @atom:B  @atom:A  and  ordered
  -> atoms @atom:A  @atom:Bt
```
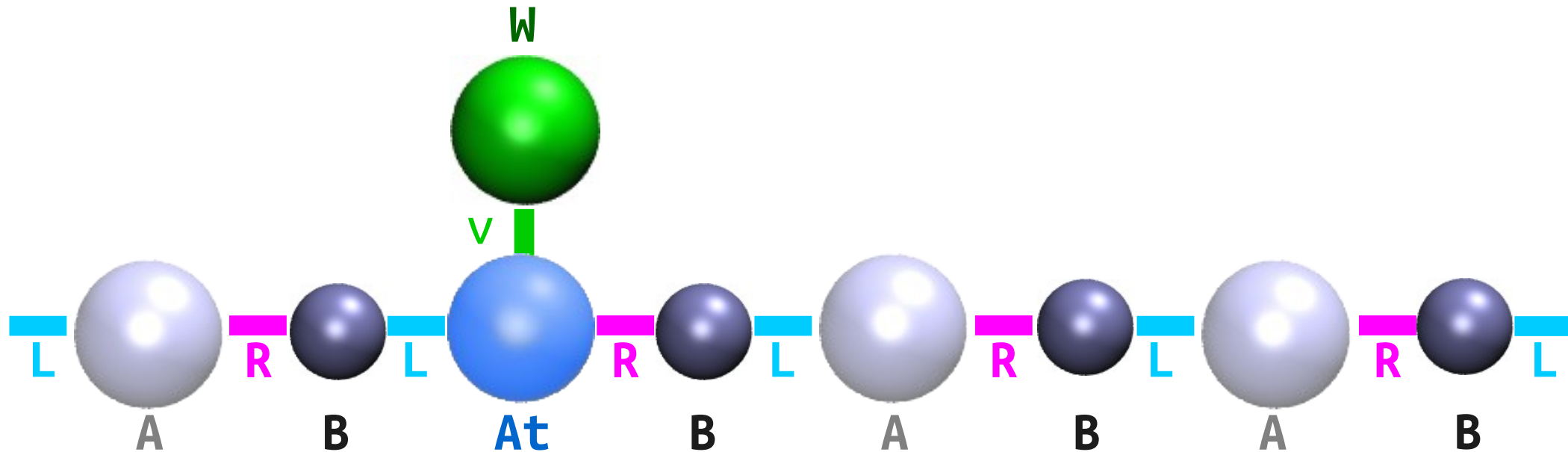
"Walker" can move right or left...

Solution Strategy: Break symmetry
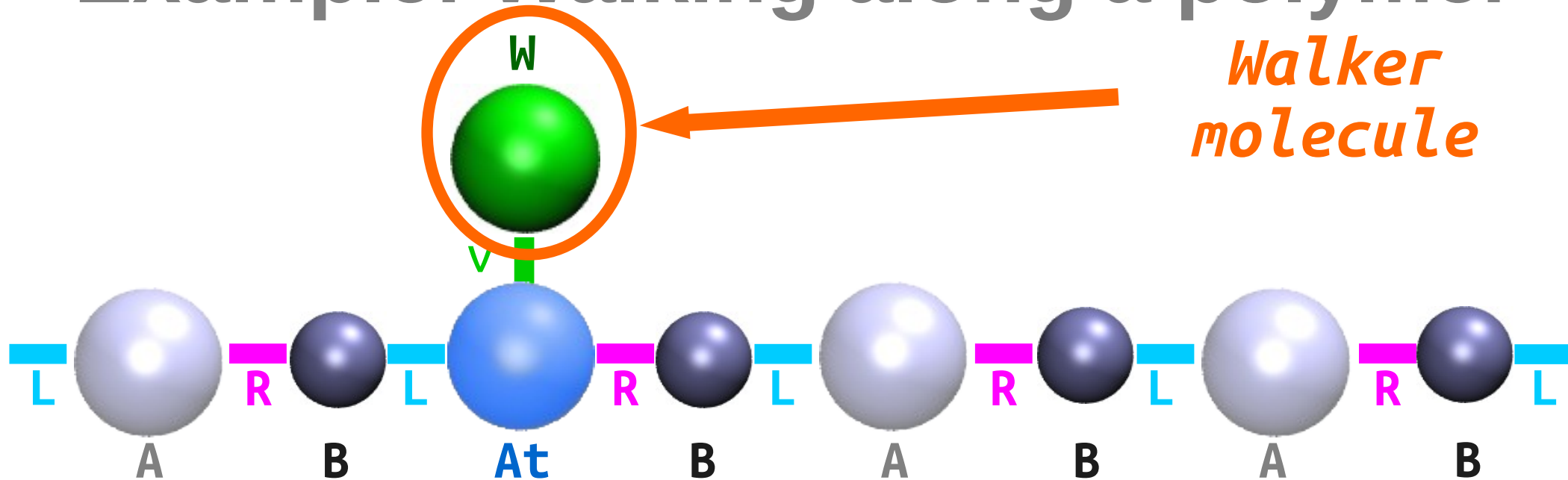## One way to do this is to use different bond types (L and R)

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
  if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
    -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
  if atoms @atom:Bt @atom:A   and  bond @bond:L
    -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
  if atoms @atom:W  @atom:AT  and  distance <= 1.5
    -> atoms @atom:Wt @atom:At  and  bond @bond:V
       and angle @angle:Ra  @atom:B @atom:Aw @atom:W
fix tr4 all bond/change 100  delay  4
  if atoms @atom:Wt @atom:A   and  bond @bond:V
    -> atoms @atom:W  @atom:A   and  bond BREAK
```

Example: Walking along a polymer
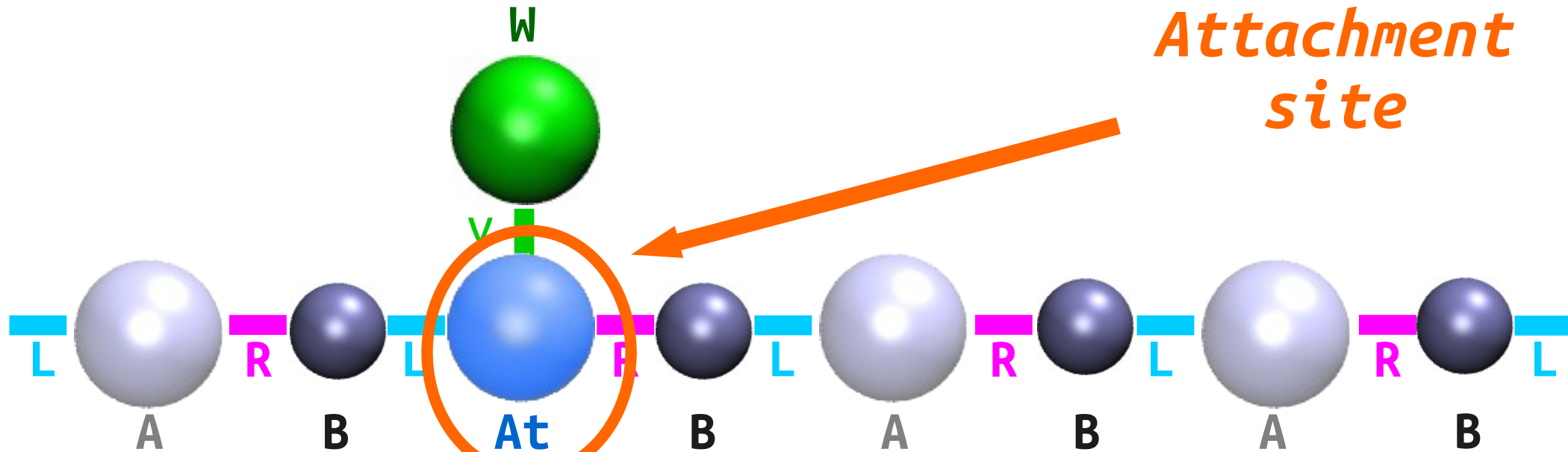

Walker molecule

```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V
        and angle @angle:Ra  @atom:B @atom:Aw @atom:W
fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```
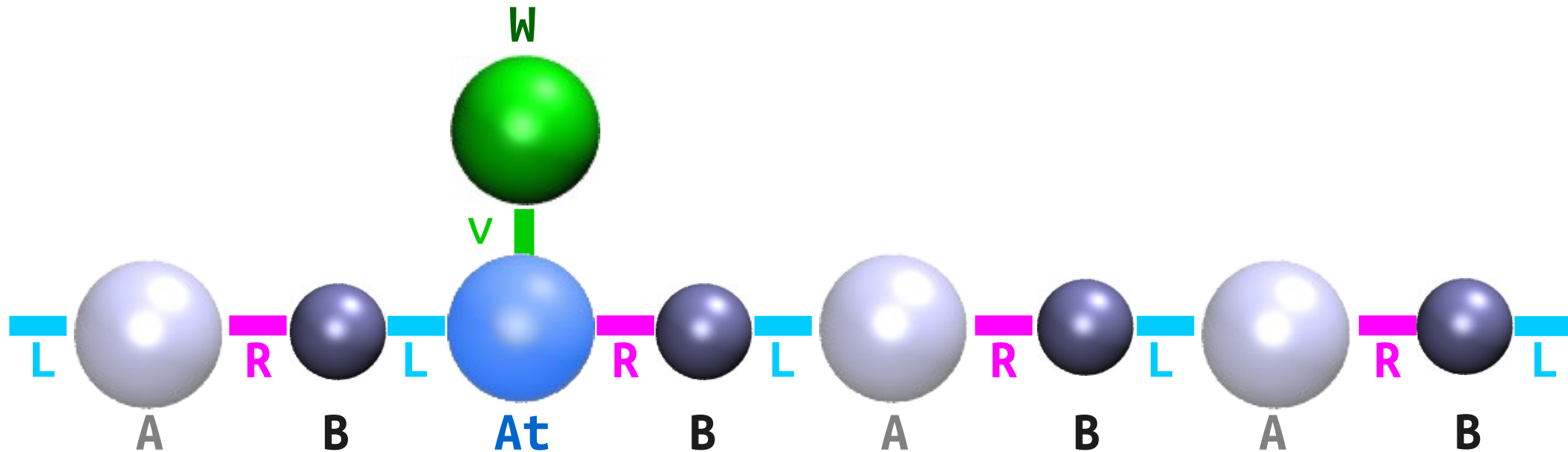
Example: Walking along a polymer
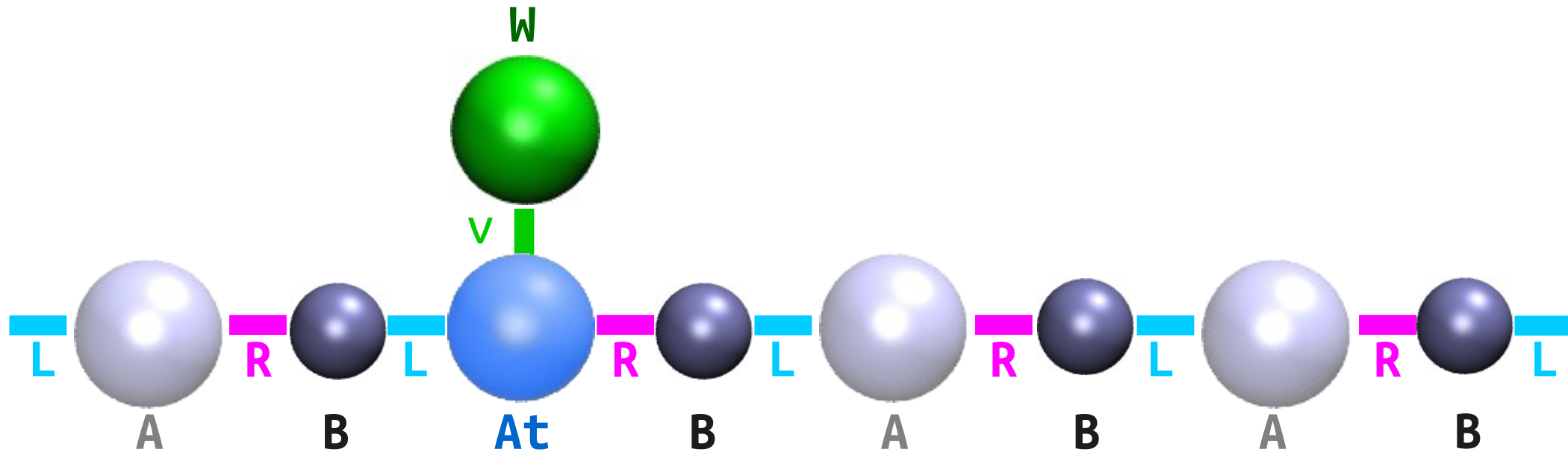

Attachment site

```
fix tr1 all bond/change 100  delay  1
  if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
  -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
  if atoms @atom:Bt @atom:A   and  bond @bond:L
  -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
  if atoms @atom:W  @atom:AT  and  distance <= 1.5
  -> atoms @atom:Wt @atom:At  and  bond @bond:V
      and angle @angle:Ra  @atom:B @atom:Aw @atom:W
fix tr4 all bond/change 100  delay  4
  if atoms @atom:Wt @atom:A   and  bond @bond:V
  -> atoms @atom:W  @atom:A   and  bond BREAK
```
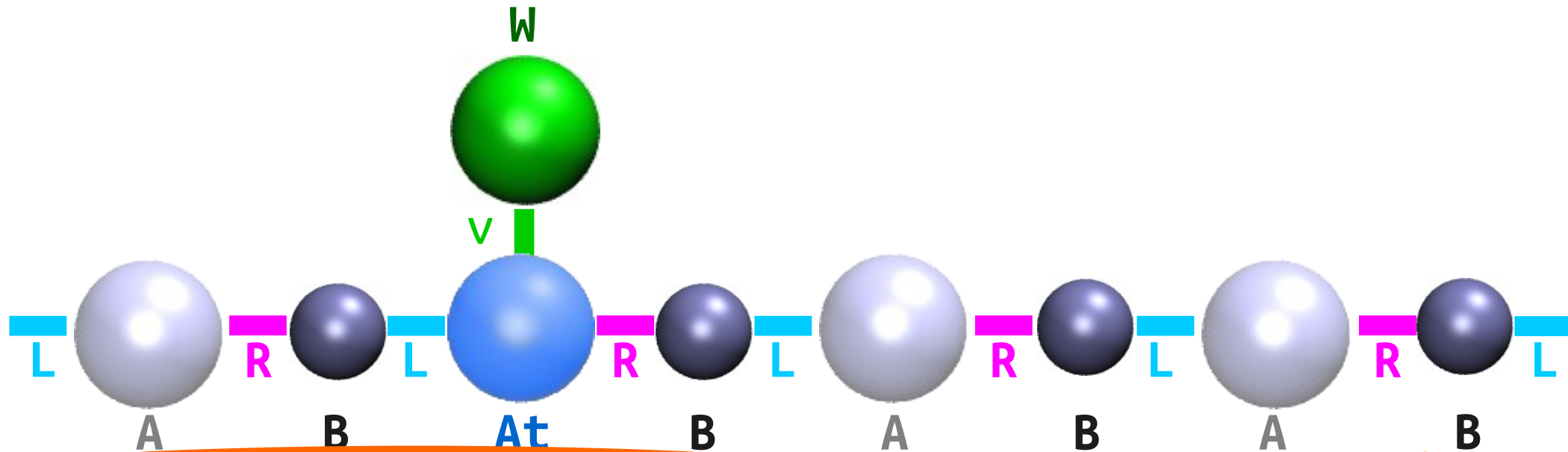
Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
  if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
  -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
  if atoms @atom:Bt @atom:A   and  bond @bond:L
  -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
  if atoms @atom:W  @atom:AT  and  distance <= 1.5
  -> atoms @atom:Wt @atom:At  and  bond @bond:V
      and angle @angle:Ra  @atom:B @atom:At @atom:W
fix tr4 all bond/change 100  delay  4
  if atoms @atom:Wt @atom:A   and  bond @bond:V
  -> atoms @atom:W  @atom:A   and  bond BREAK
```

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B    and   bond @bond:R   and   prob 0.2
   -> atoms @atom:A   @atom:Bt
```
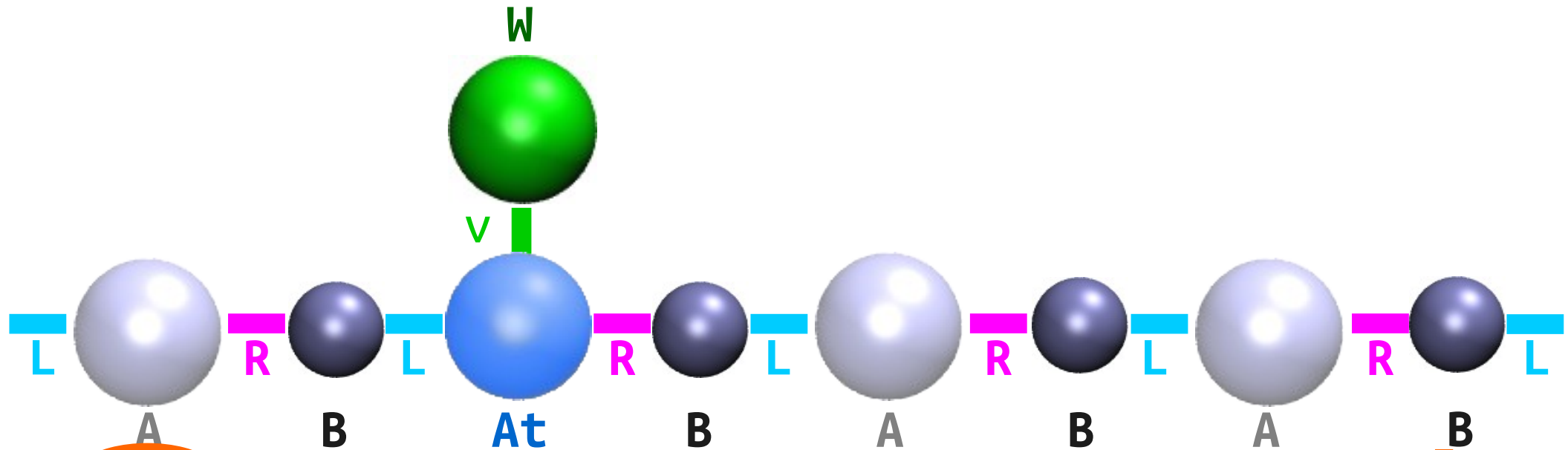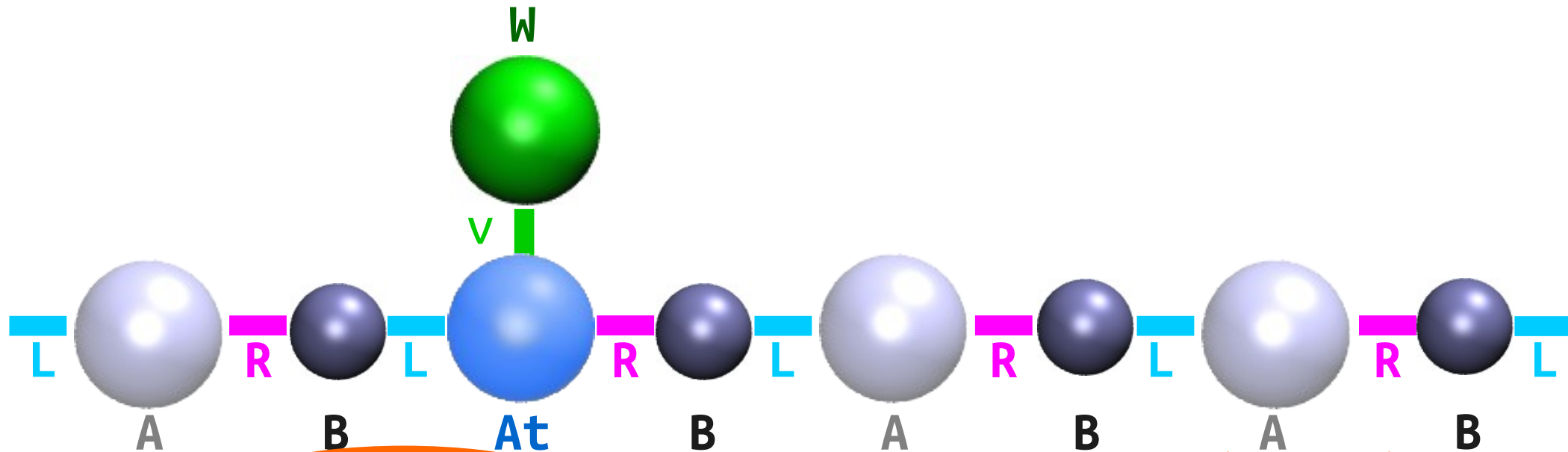
Example: Walking along a polymer

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay 1
  if atoms @atom:At @atom:B  and  bond @bond:R
  -> atoms @atom:A  @atom:Bt
```

Must supply a unique name for each command (eg. "tr1" Sorry, this is a LAMMPS requirement)
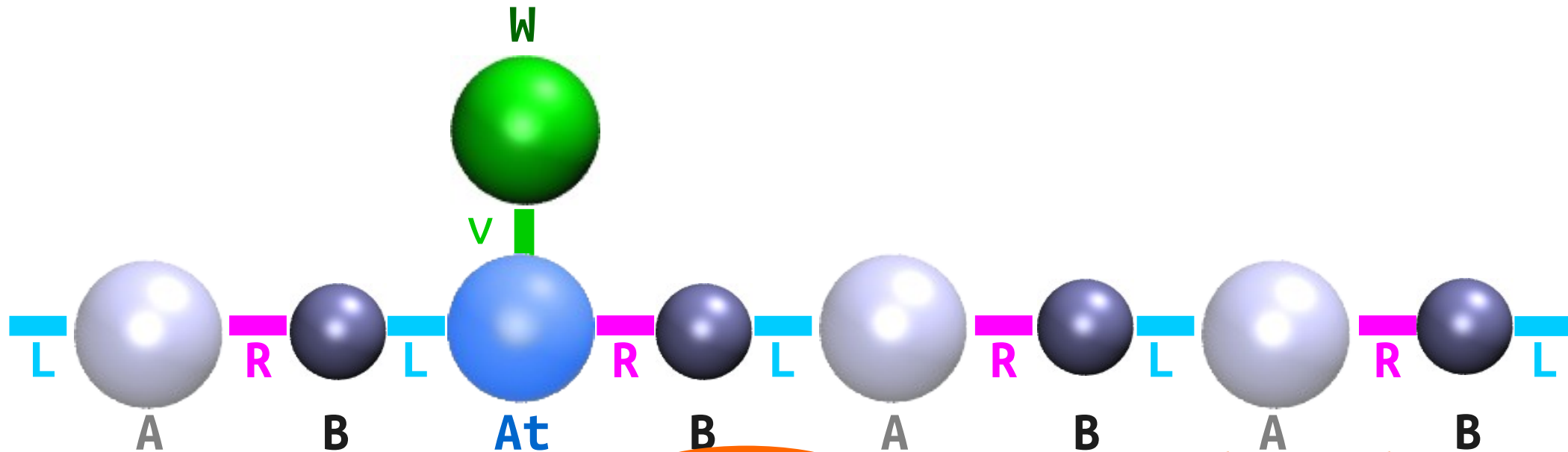
Example: Walking along a polymer


```
fix tr1 all bond/change 100 delay 1
  if atoms @atom:At @atom:B   and  bond @bond:R
  -> atoms @atom:A  @atom:Bt
```

What do you want to do?

(modify an existing bond)
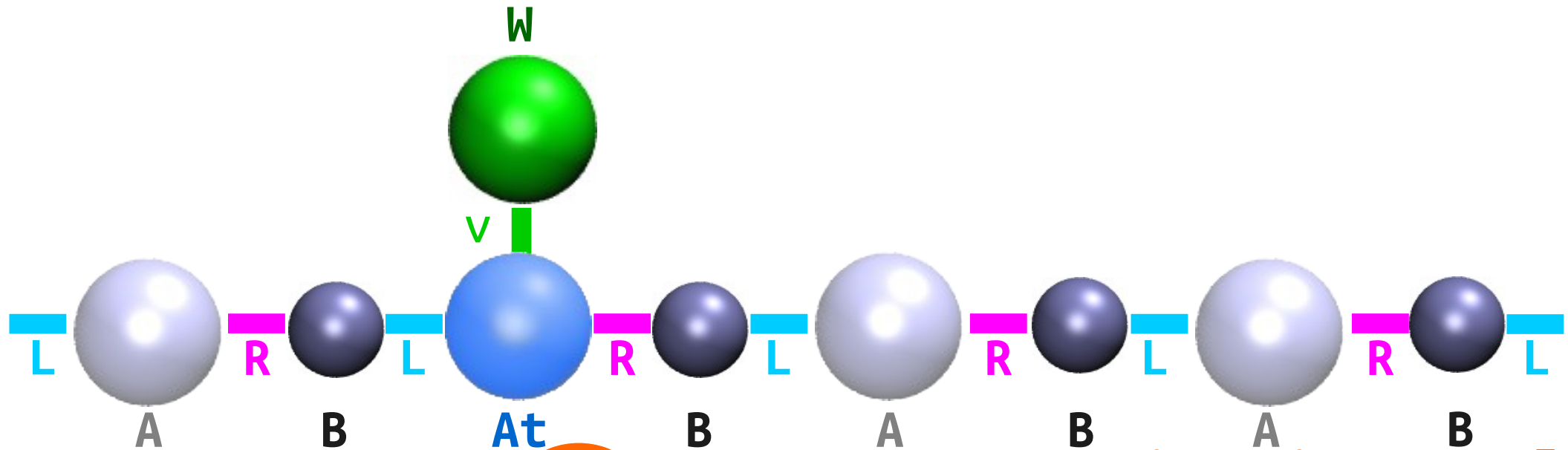
Example: Walking along a polymer


```
fix tr1 all bond/change 100   delay  1
  if atoms @atom:At @atom:B    and  bond @bond:R
  -> atoms @atom:A  @atom:Bt
```

When do you want to do it?
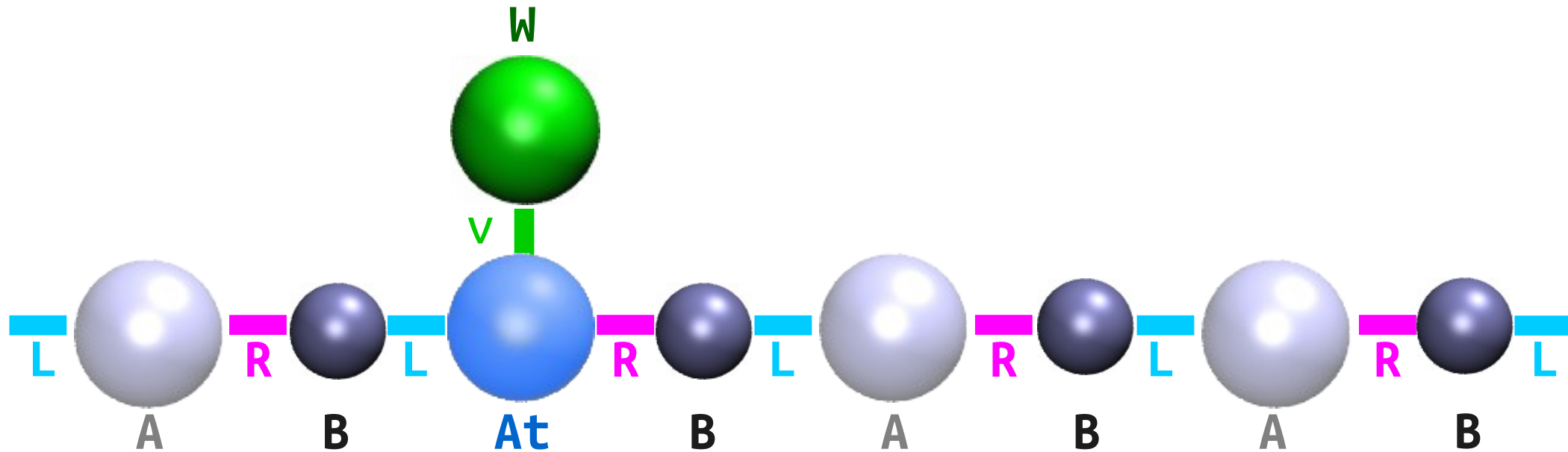
(similar to a "line number")

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay 1
  if atoms @atom:At @atom:B   and  bond @bond:R
  -> atoms @atom:A  @atom:Bt
```
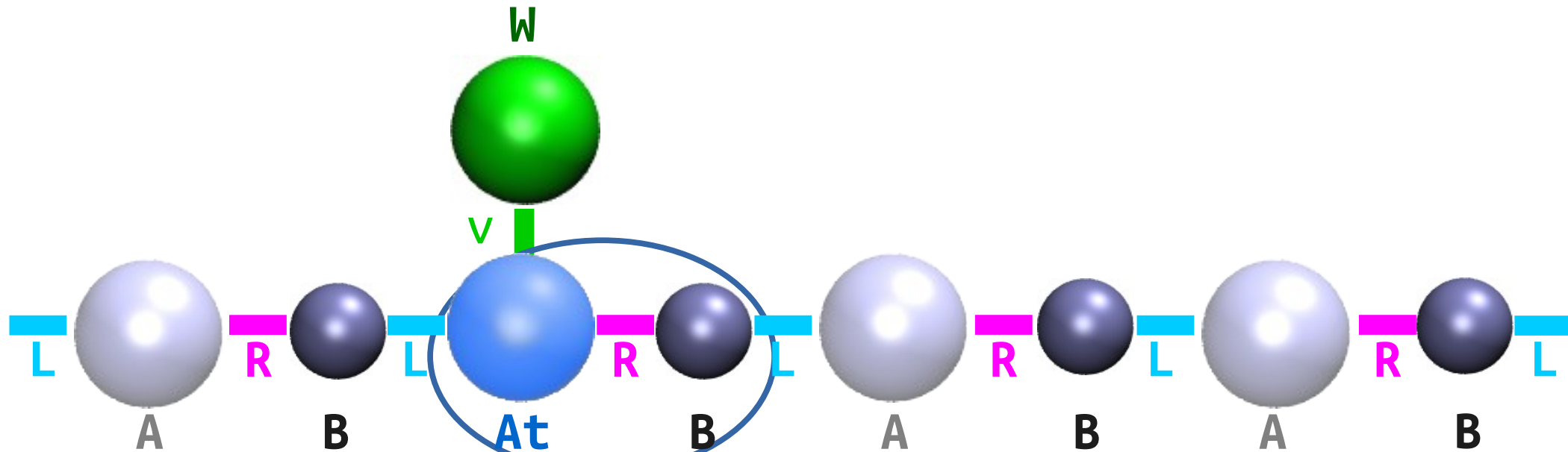
Time interval (in MD timesteps) between cycles of logic transitions

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
```

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
  if atoms @atom:At @atom:B    and  bond @bond:R  and  prob 0.2
  -> atoms @atom:A  @atom:Bt
```
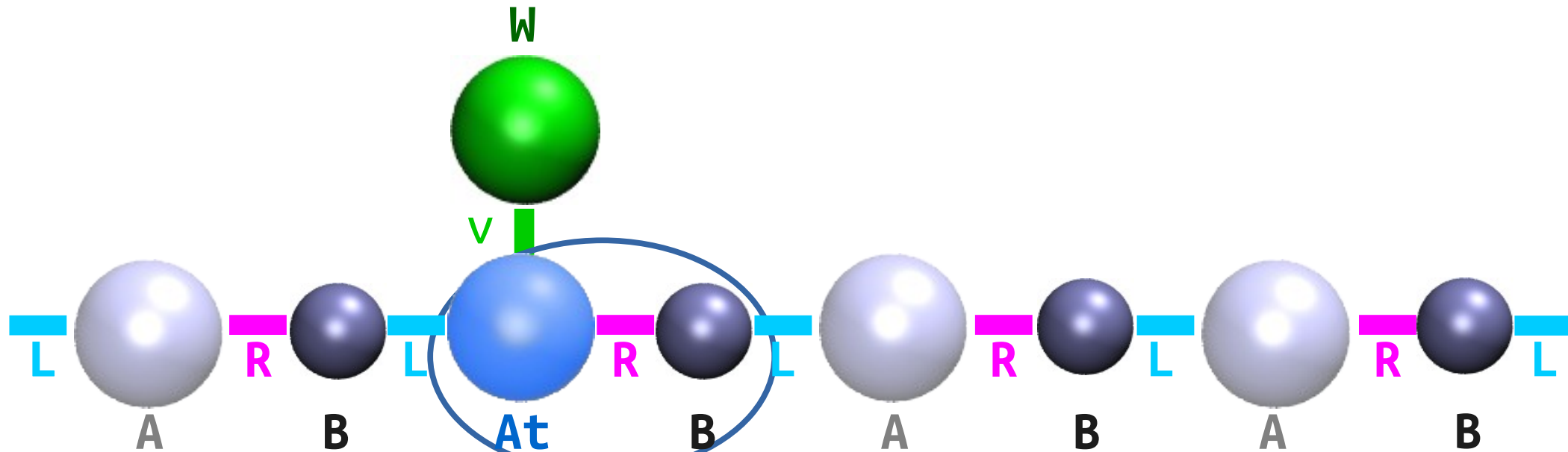
Example: Walking along a polymer
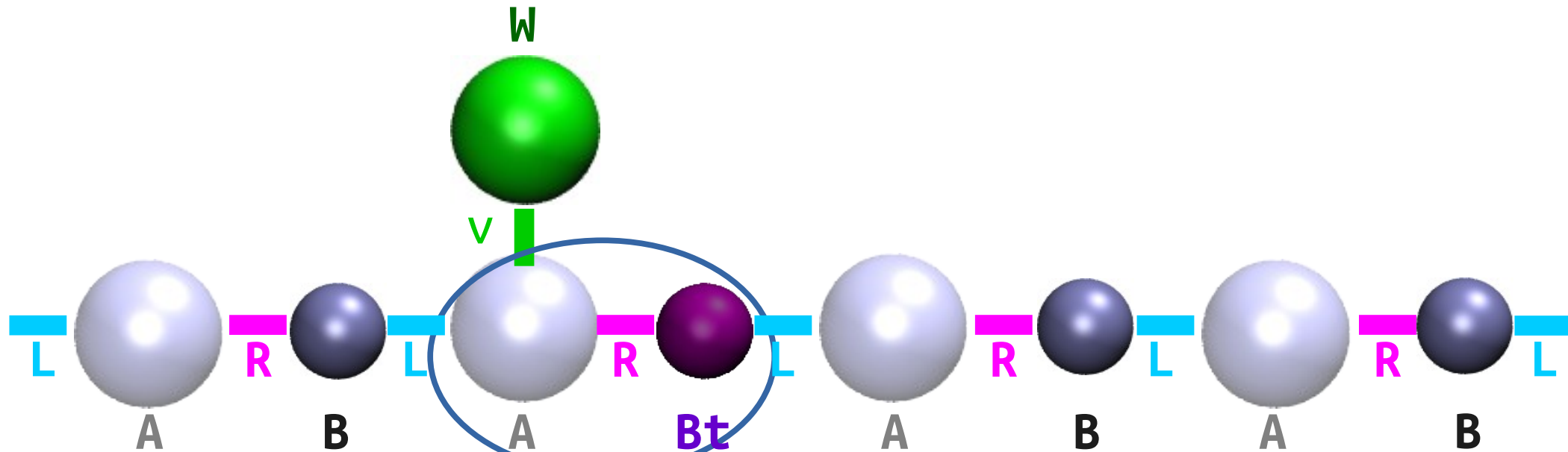


```
fix tr1 all bond/change 100  delay  1
  if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
  -> atoms @atom:A  @atom:Bt
```

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
  if atoms @atom:At @atom:B    and  bond @bond:R  and  prob 0.2
  -> atoms @atom:A   @atom:Bt
```

Example: Walking along a polymer
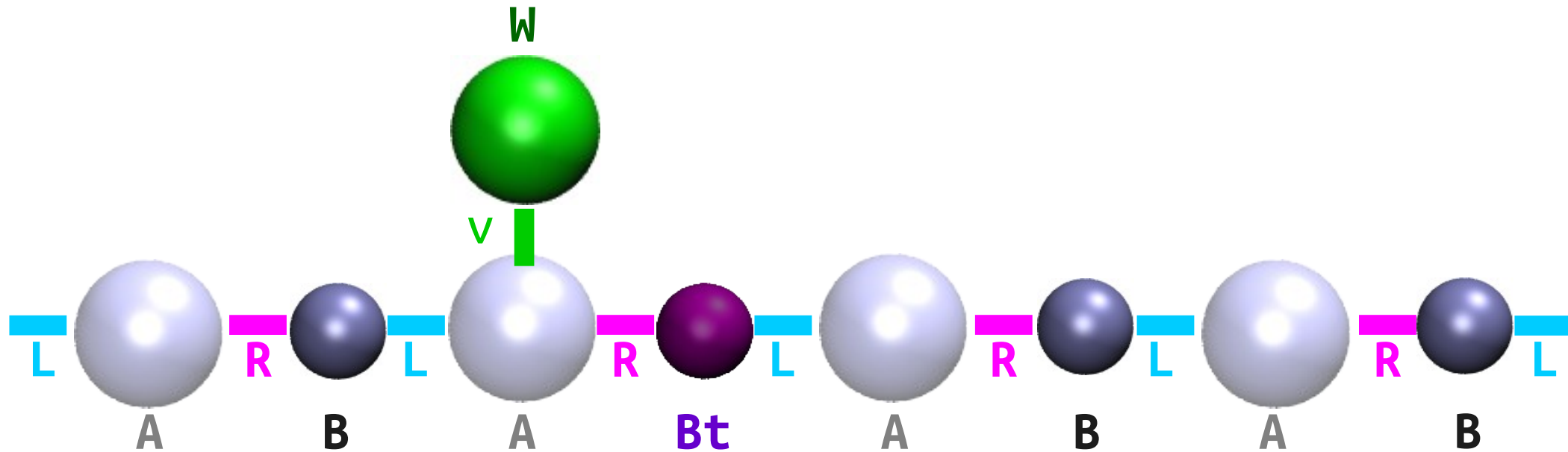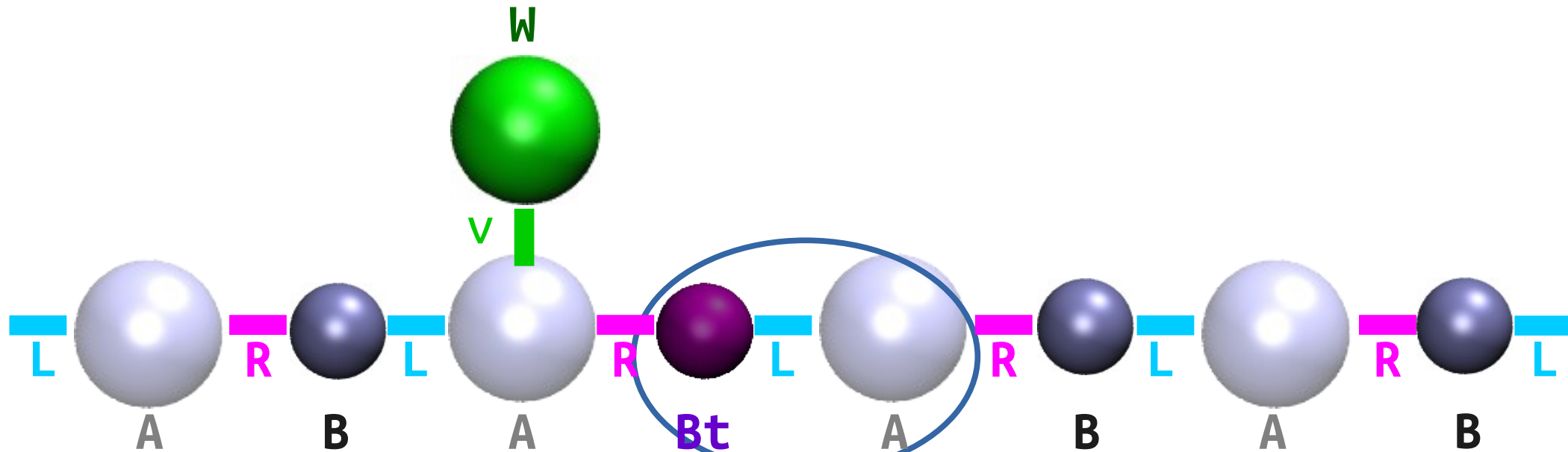


```
fix tr1 all bond/change 100  delay  1
  if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
  -> atoms @atom:A  @atom:Bt
```

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B    and   bond @bond:R  and   prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A    and   bond @bond:L
   -> atoms @atom:B  @atom:Al
```
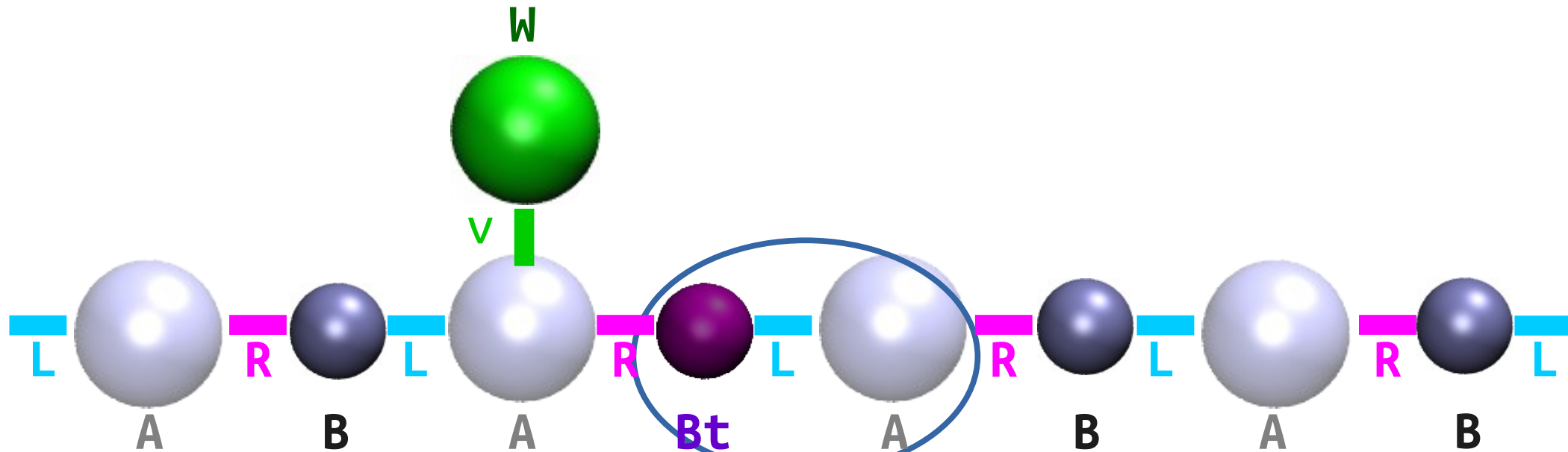
Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B    and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A    and  bond @bond:L
   -> atoms @atom:B  @atom:AT
```
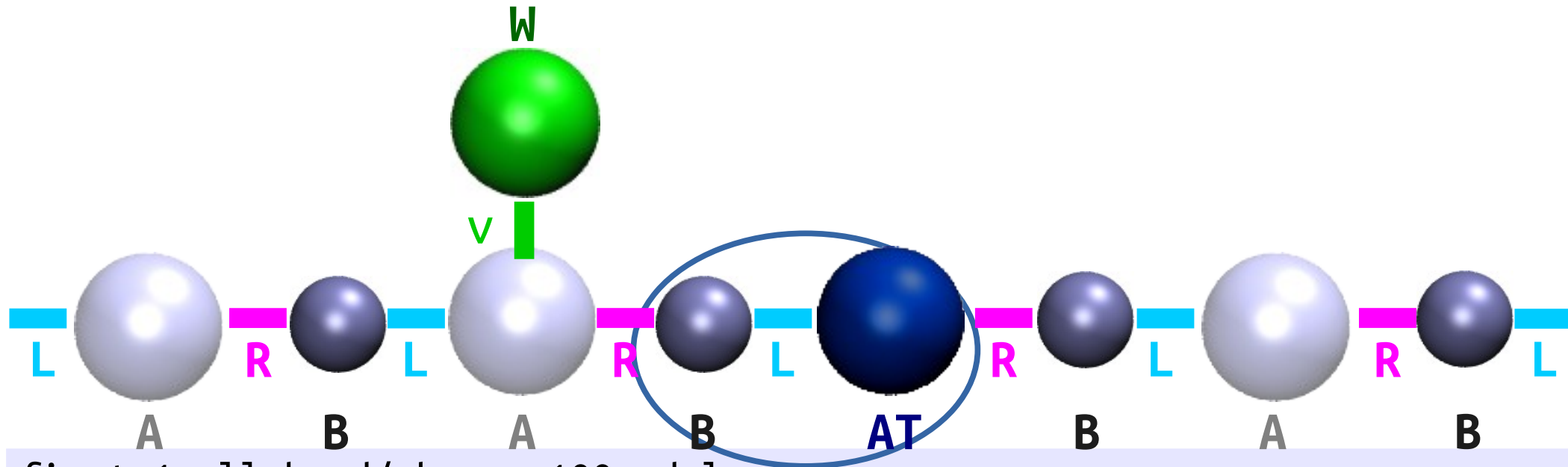
Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A    and  bond @bond:L
   -> atoms @atom:B  @atom:AT
```
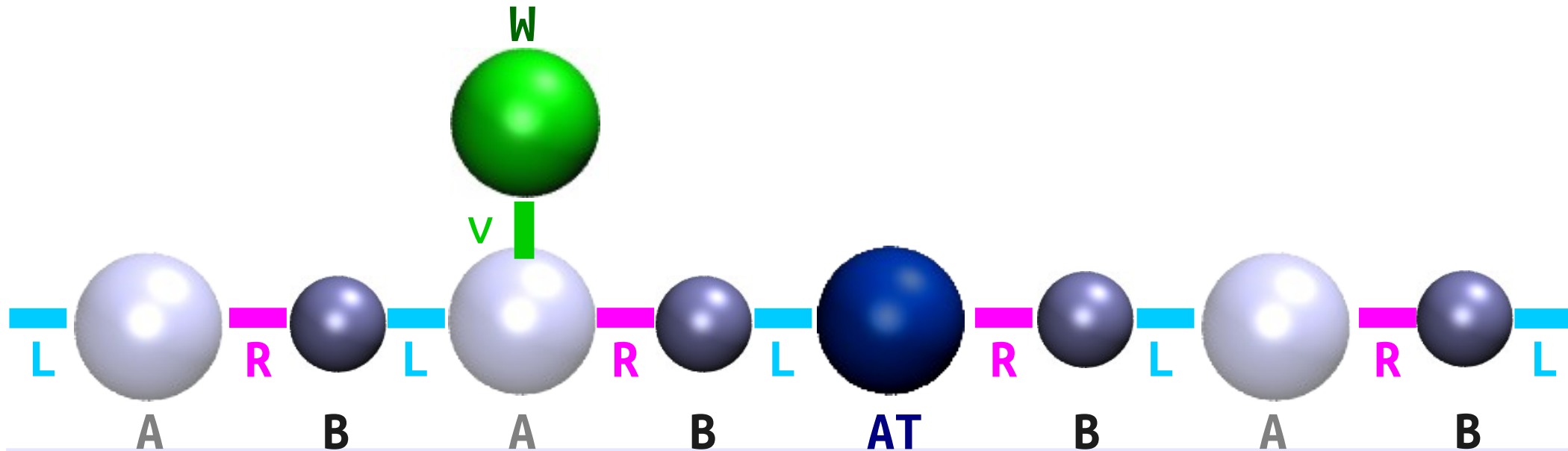
Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
```
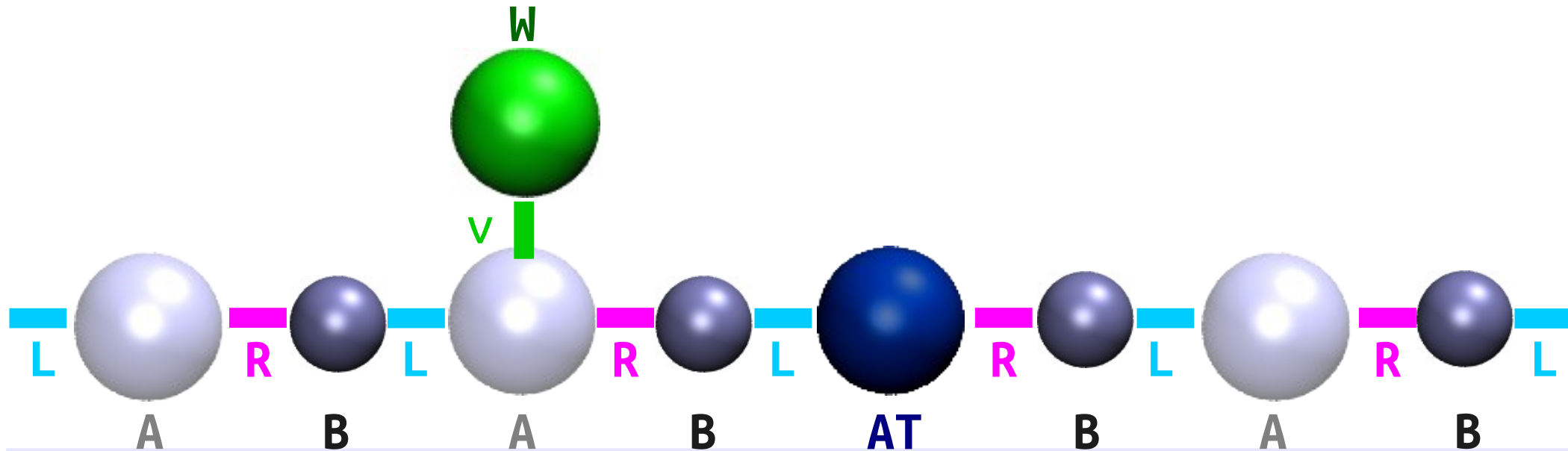
Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
  if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
  -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
  if atoms @atom:Bt @atom:A   and  bond @bond:L
  -> atoms @atom:B  @atom:AT
fix tr3 all bond/new     100  delay  3
  if atoms @atom:W  @atom:AT  and  distance <= 1.5
  -> atoms @atom:Wt @atom:At  and  bond @bond:V
```

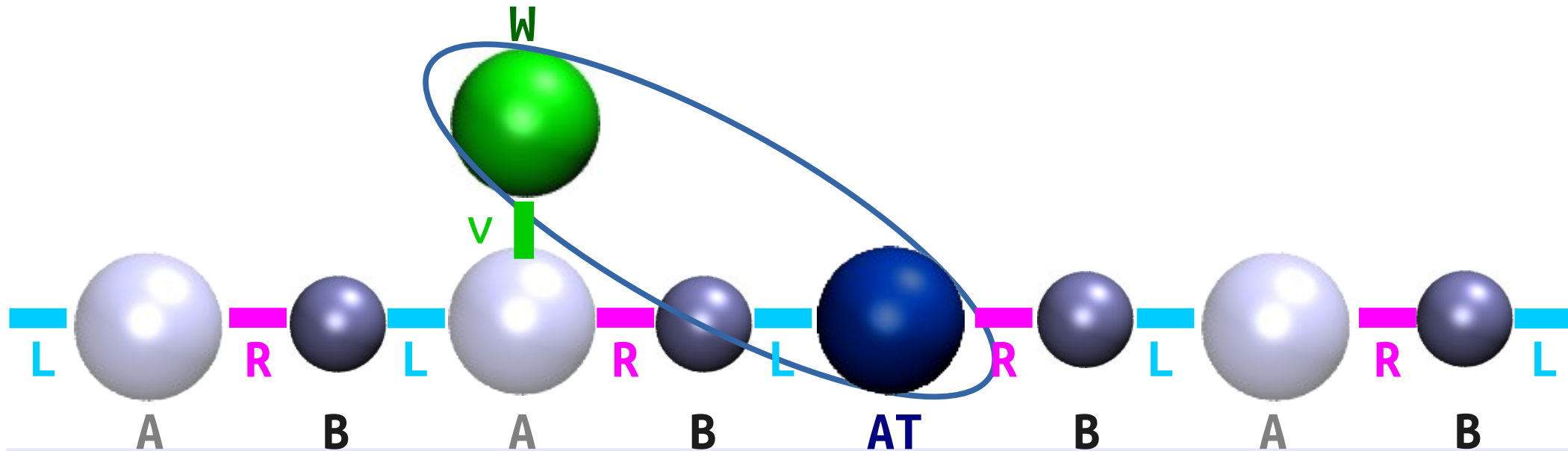# Example: Walking along a polymer
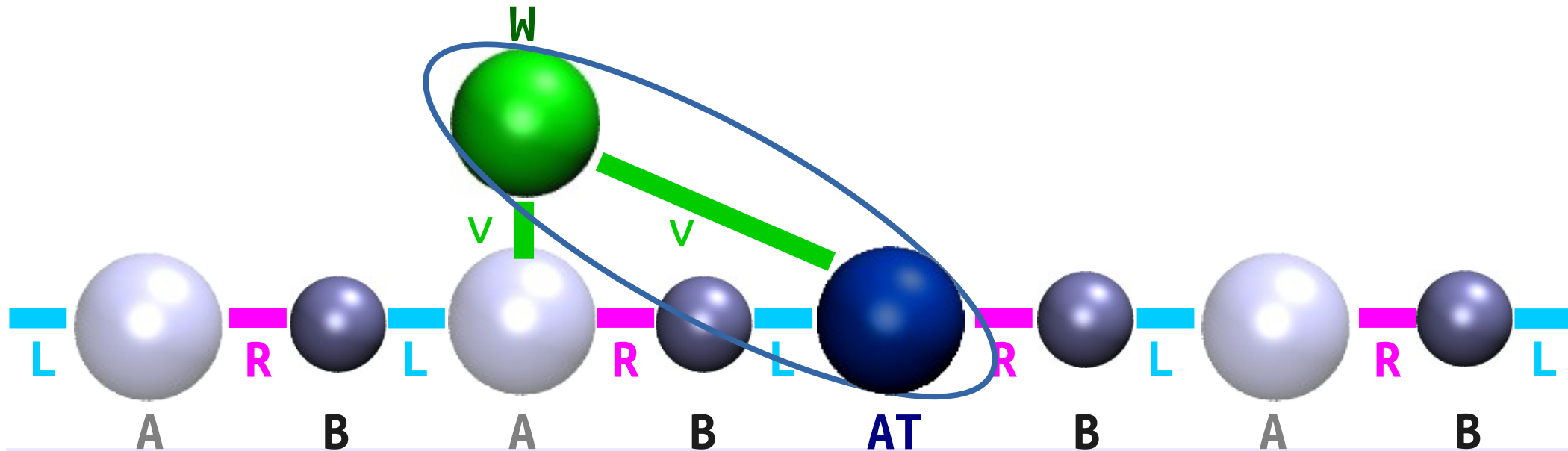


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new     100  delay  3
   if atoms @atom:W  @atom:AT  and   distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V
```

Example: Walking along a polymer
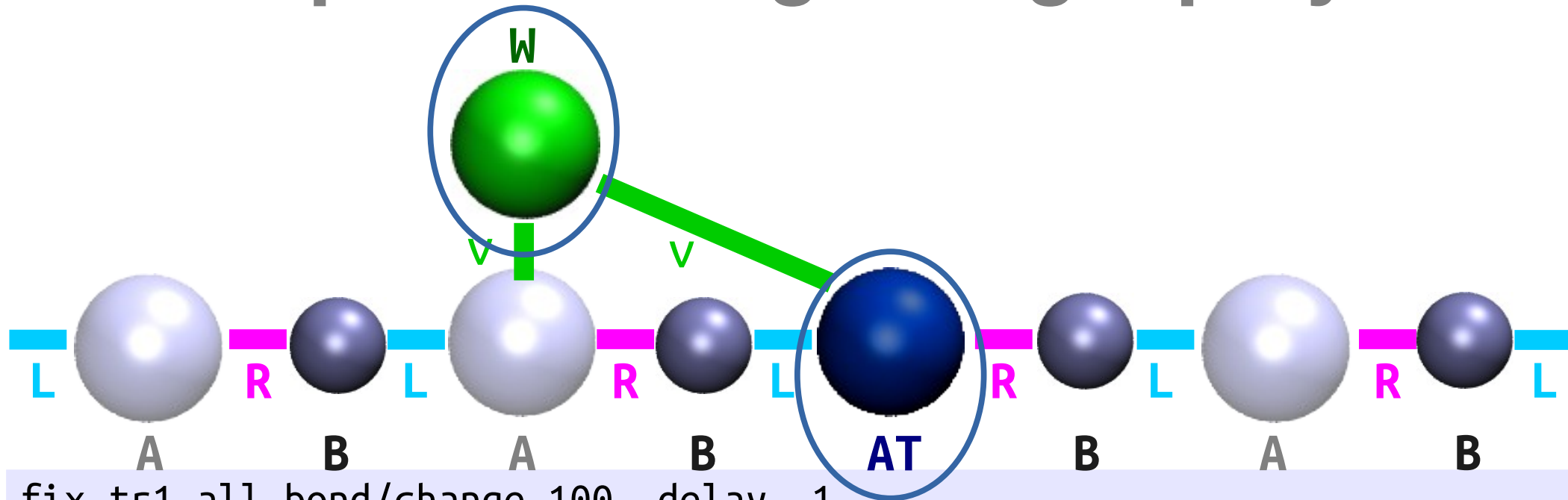


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and   distance <= 1.5
   -> atoms @atom:Wt @atom:At  and   bond @bond:V
```

Example: Walking along a polymer
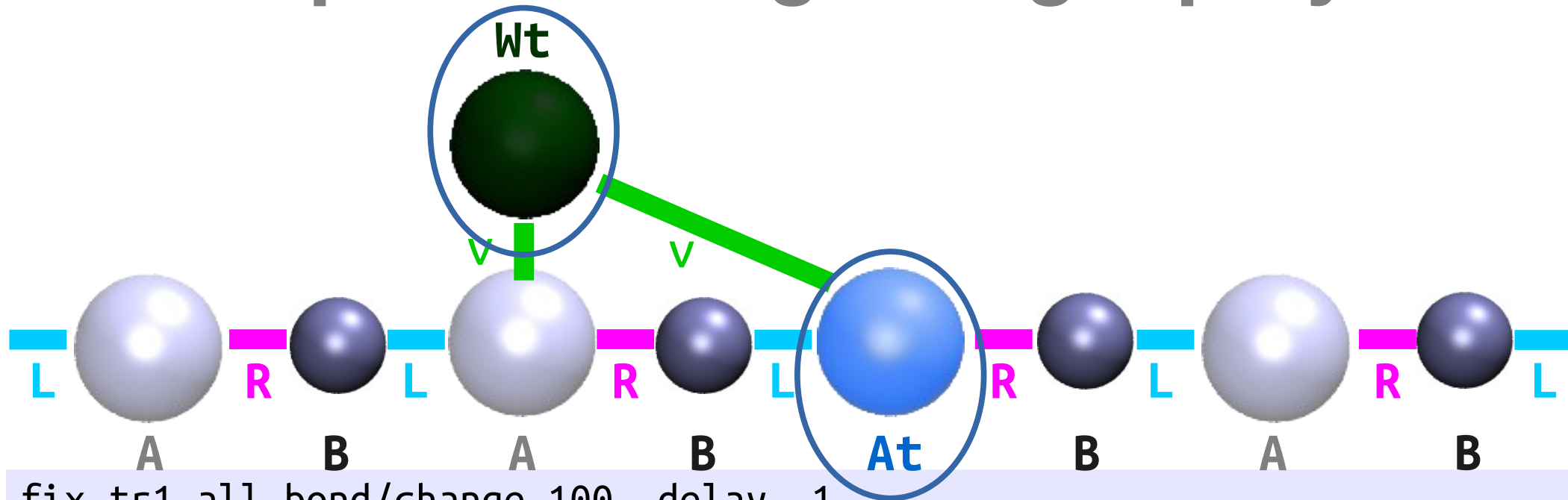


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B    and   bond @bond:R   and   prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A    and   bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new     100  delay  3
   if atoms @atom:W  @atom:AT   and   distance <= 1.5
   -> atoms @atom:Wt @atom:At   and   bond @bond:V
```
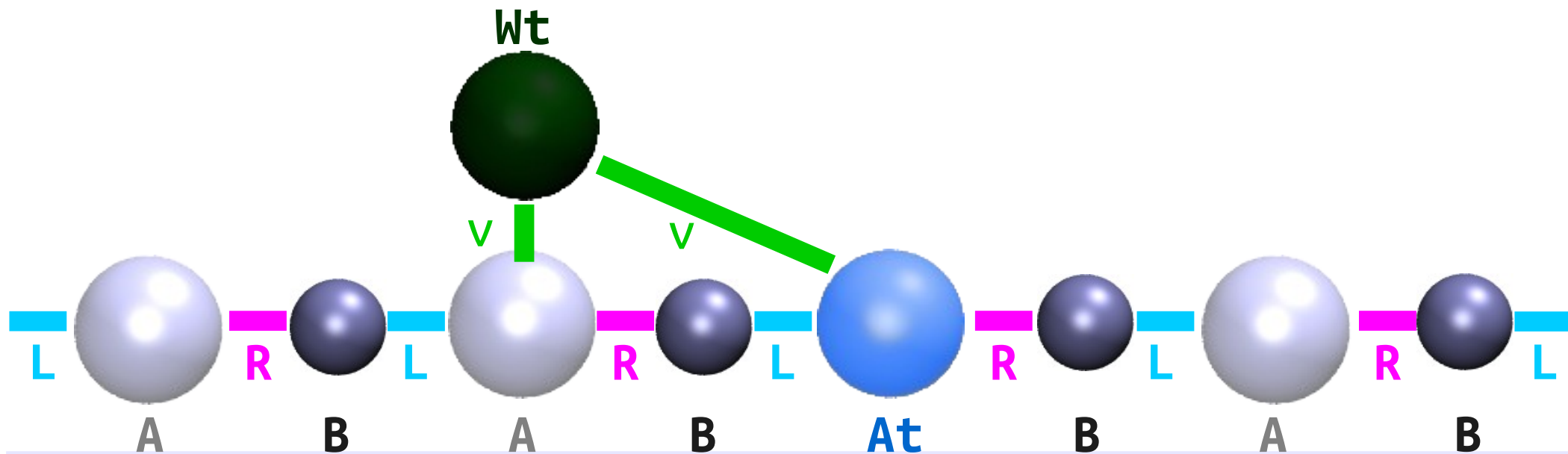
Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and   bond @bond:R  and   prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and   bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and   distance <= 1.5
   -> atoms @atom:Wt @atom:At  and   bond @bond:V
```

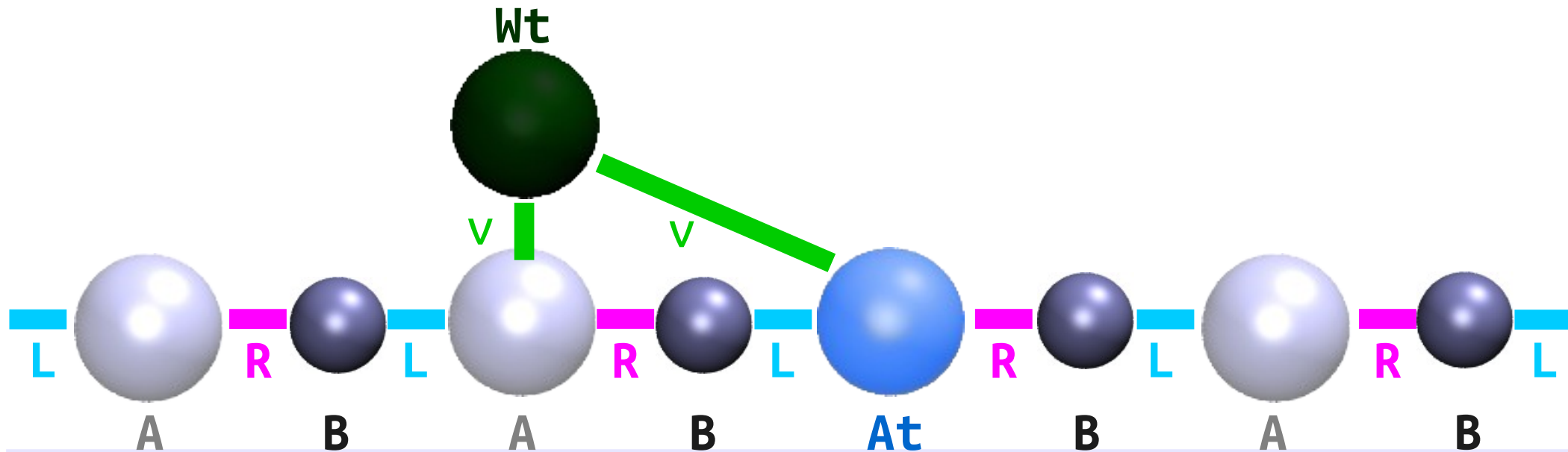# Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
  if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
  -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
  if atoms @atom:Bt @atom:A   and  bond @bond:L
  -> atoms @atom:B  @atom:AT
fix tr3 all bond/new     100  delay  3
  if atoms @atom:W  @atom:AT  and  distance <= 1.5
  -> atoms @atom:Wt @atom:At  and  bond @bond:V
```

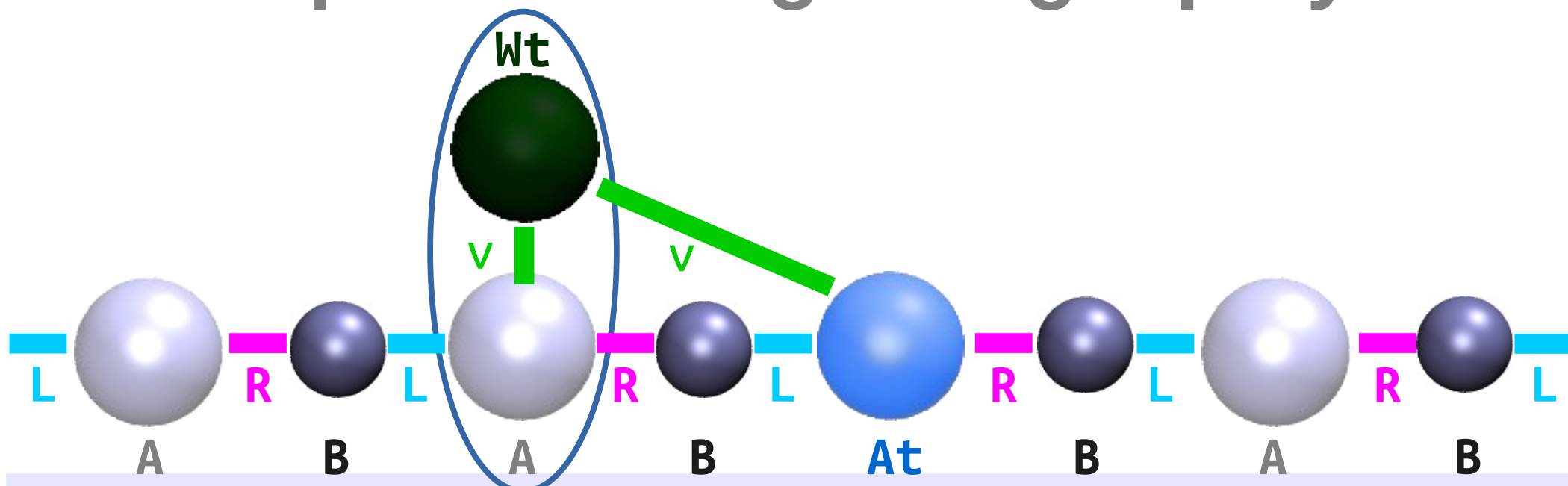# Example: Walking along a polymer
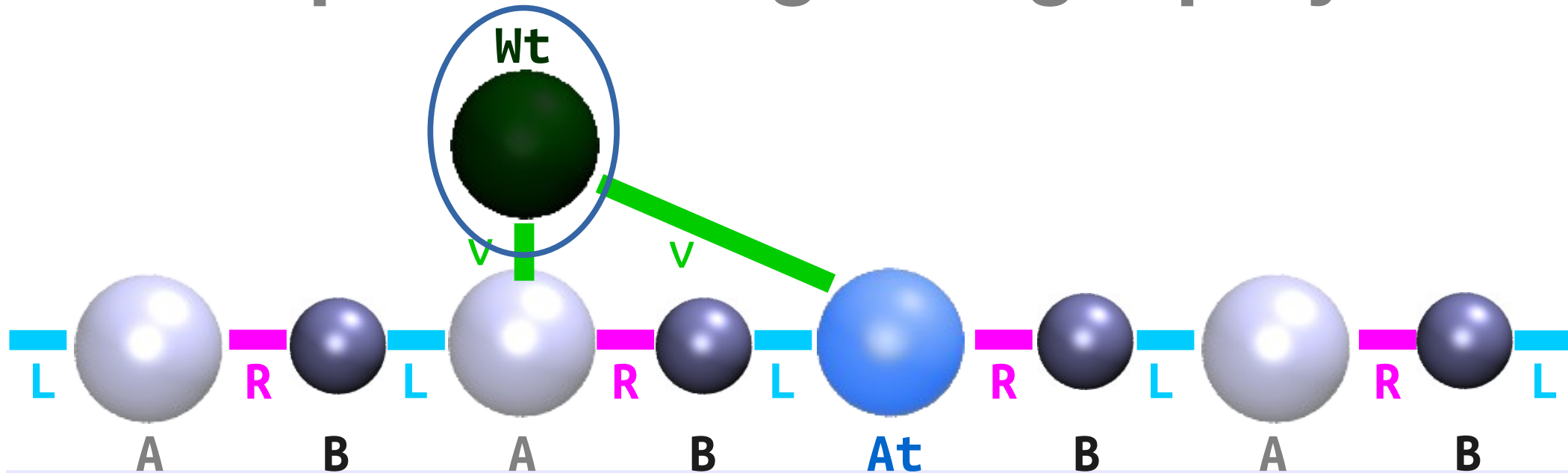


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new     100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V

fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```

Example: Walking along a polymer
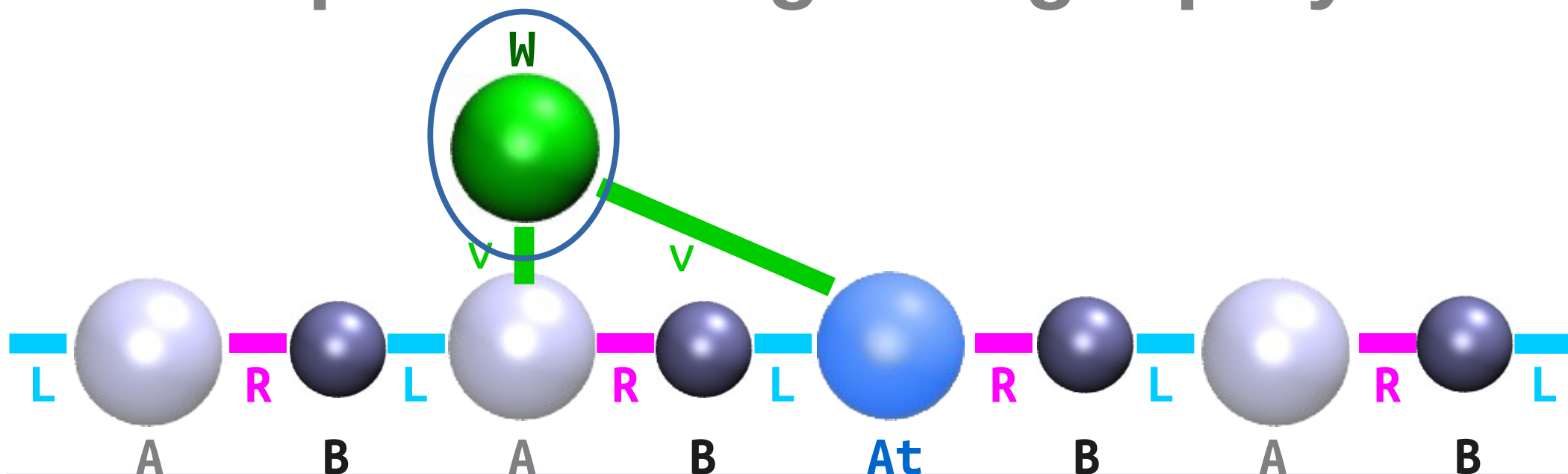


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V

fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and   bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new     100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V

fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```
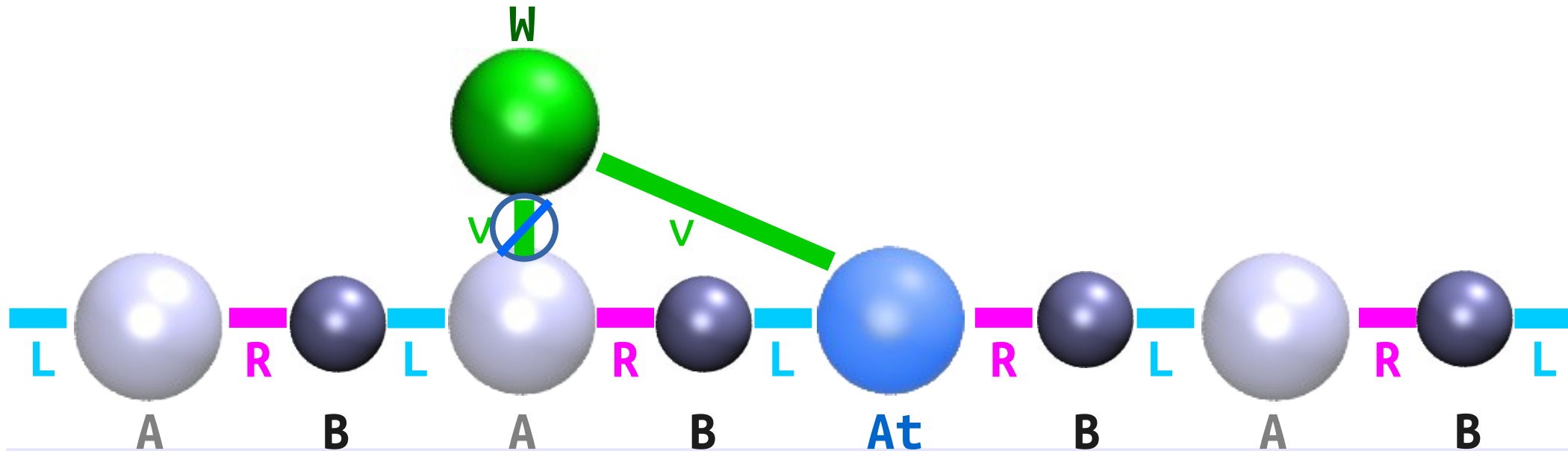
Example: Walking along a polymer


```
fix tr1 all bond/change 100   delay  1
   if atoms @atom:At @atom:B    and   bond @bond:R   and   prob 0.2
   -> atoms @atom:A   @atom:Bt
fix tr2 all bond/change 100   delay  2
   if atoms @atom:Bt @atom:A    and   bond @bond:L
   -> atoms @atom:B   @atom:AT
fix tr3 all bond/new     100   delay  3
   if atoms @atom:W   @atom:AT   and   distance <= 1.5
   -> atoms @atom:Wt  @atom:At   and   bond @bond:V

fix tr4 all bond/change 100   delay  4
   if atoms @atom:Wt  @atom:A    and   bond @bond:V
   -> atoms @atom:W   @atom:A    and   bond BREAK
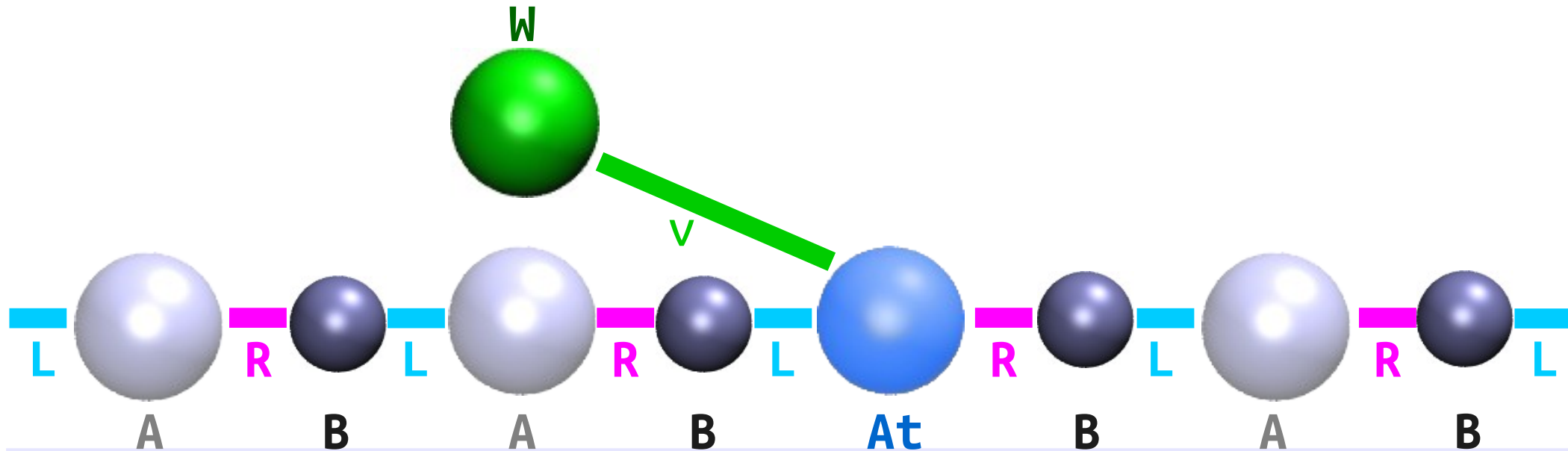```
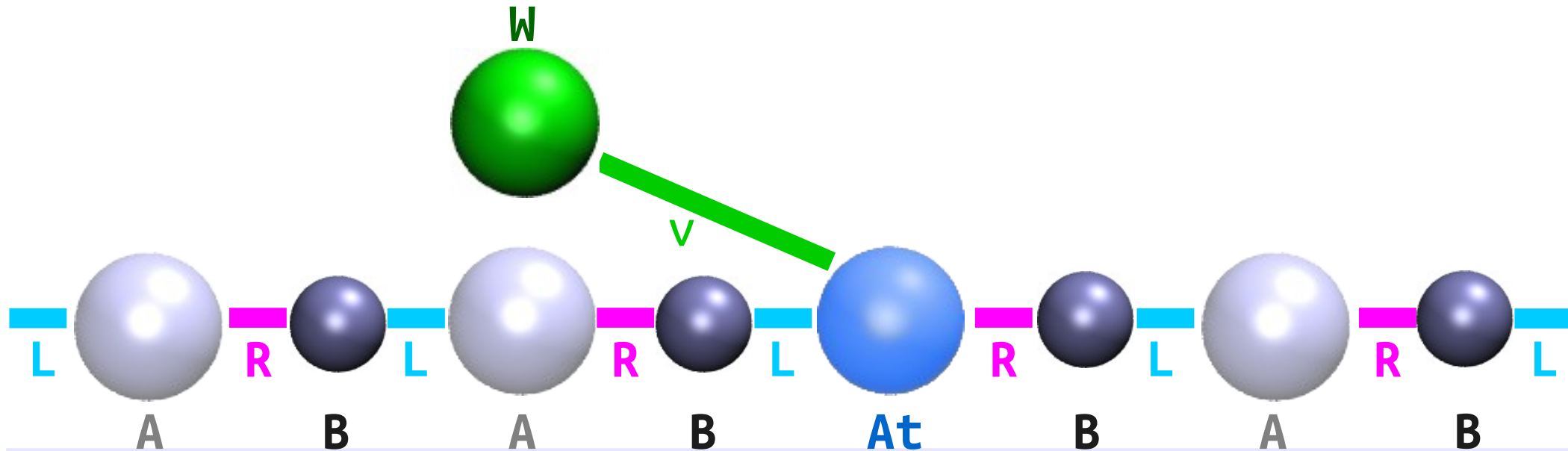
# Example: Walking along a polymer



```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V

fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```

Example: Walking along a polymer
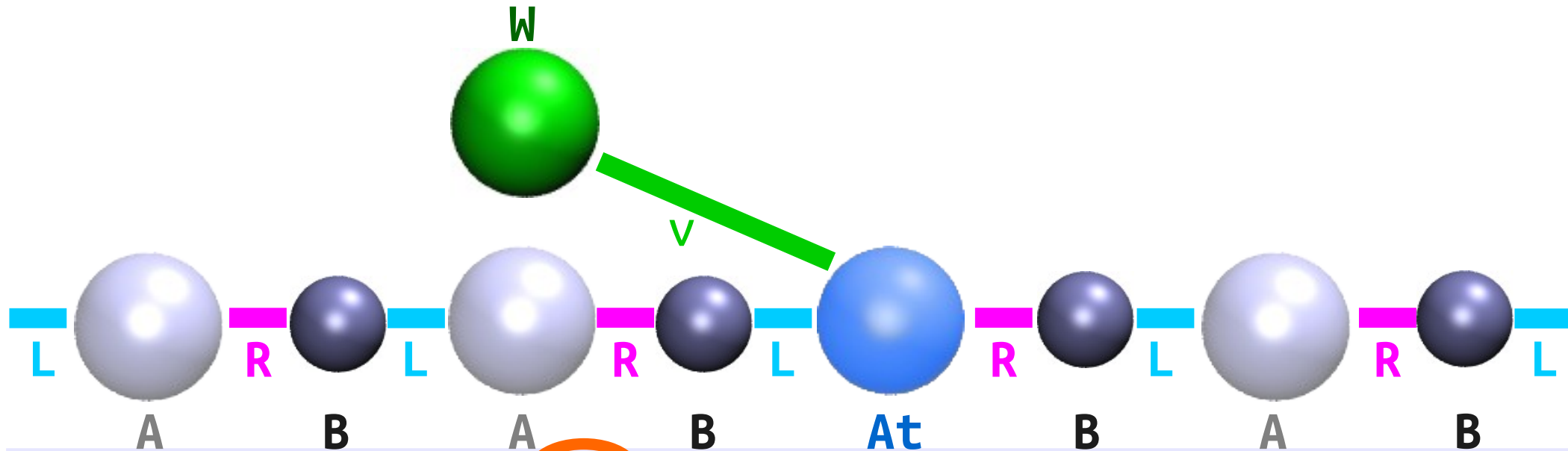


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V

fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```

Example: Walking along a polymer
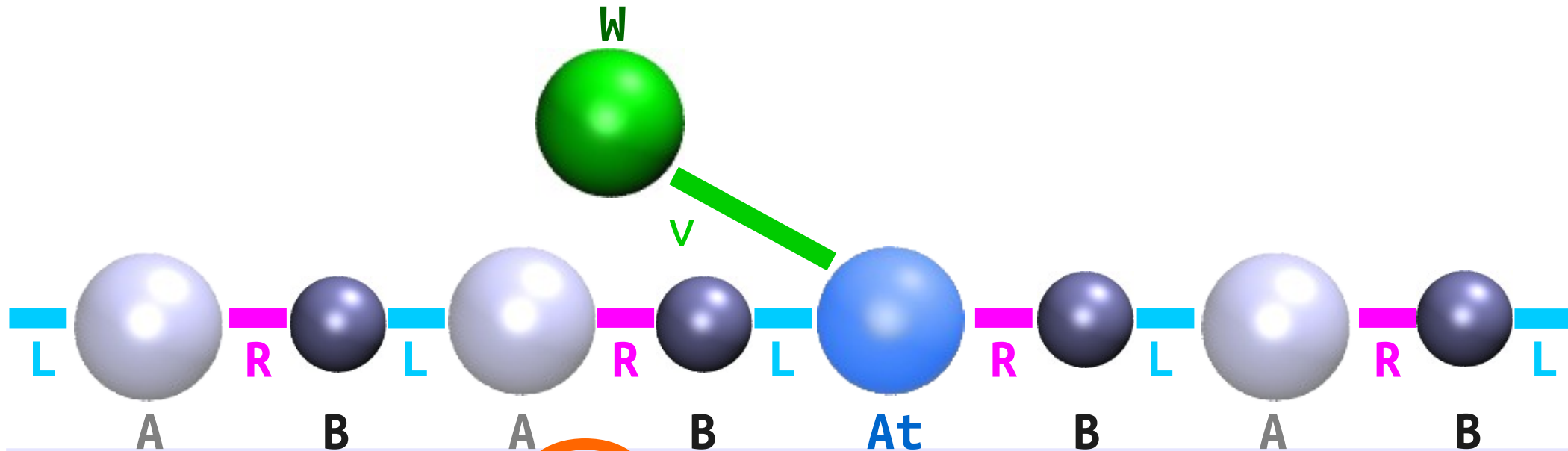


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V

fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```
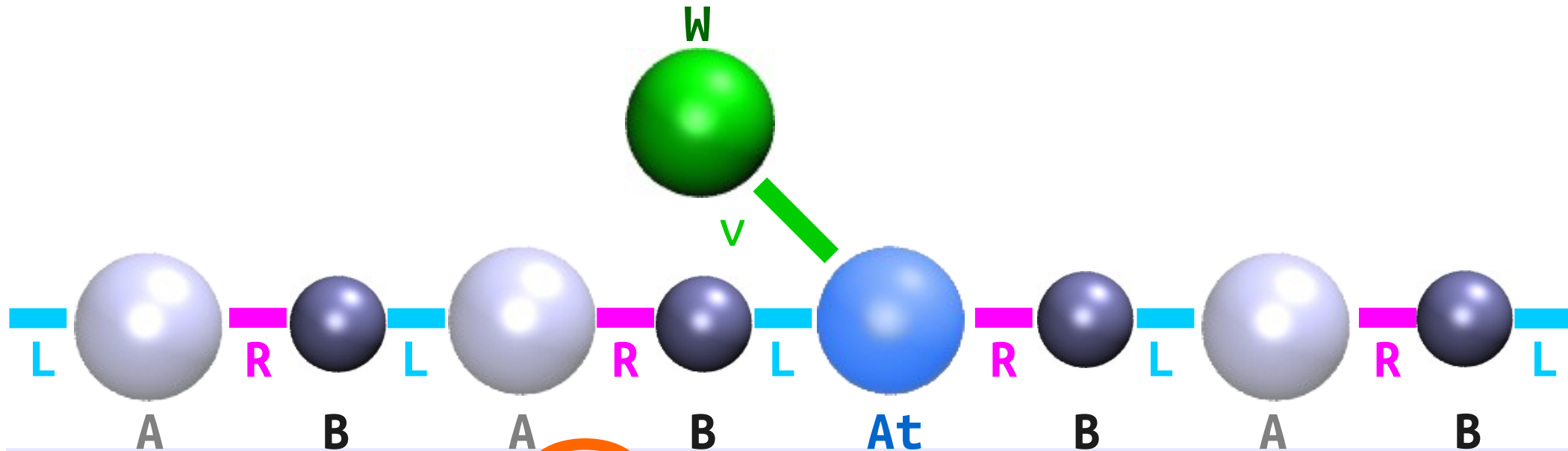
Example: Walking along a polymer


```
fix tr1 all bond/change 100 delay 1
  if atoms @atom:At @atom:B    and  bond @bond:R  and  prob 0.2
  -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100 delay 2
  if atoms @atom:Bt @atom:A    and  bond @bond:L
  -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100 delay 3
  if atoms @atom:W  @atom:AT   and  distance <= 1.5
  -> atoms @atom:Wt @atom:At   and  bond @bond:V

fix tr4 all bond/change 100 delay 4
  if atoms @atom:Wt @atom:A    and  bond @bond:V
  -> atoms @atom:W  @atom:A    and  bond BREAK
```

NOW RUN MOLECULAR DYNAMICS
(100 Verlet steps)

(Allow particles to move)

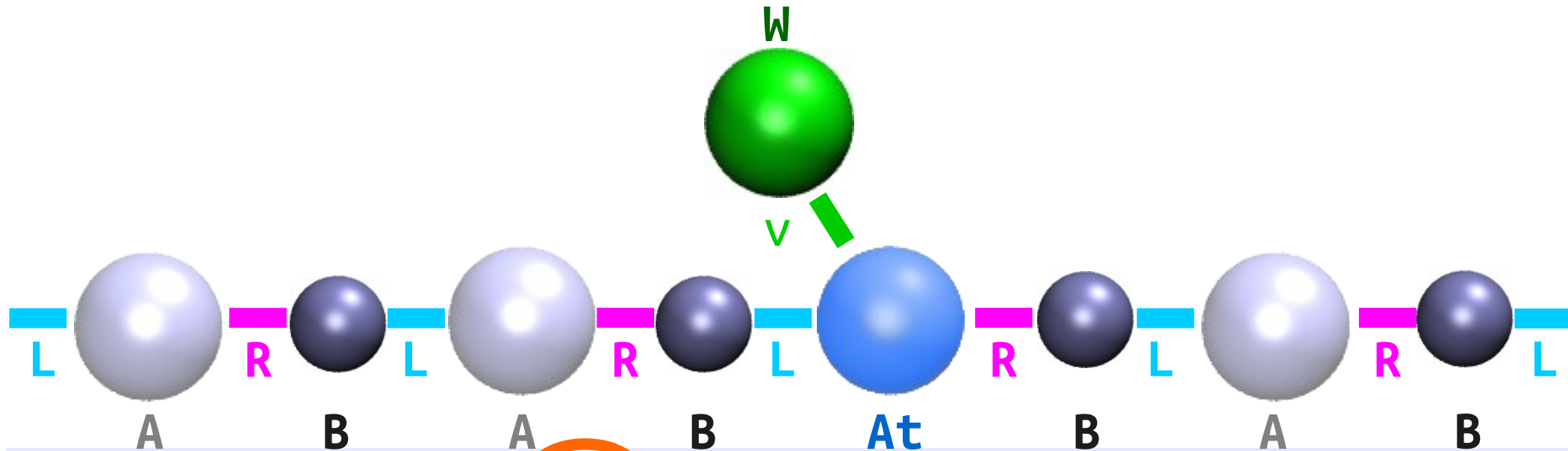# Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B    and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A    and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT   and  distance <= 1.5
   -> atoms @atom:Wt @atom:At   and  bond @bond:V

fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A    and  bond @bond:V
   -> atoms @atom:W  @atom:A    and  bond BREAK
```

NOW RUN MOLECULAR DYNAMICS
(100 Verlet steps)

(Allow particles to move)
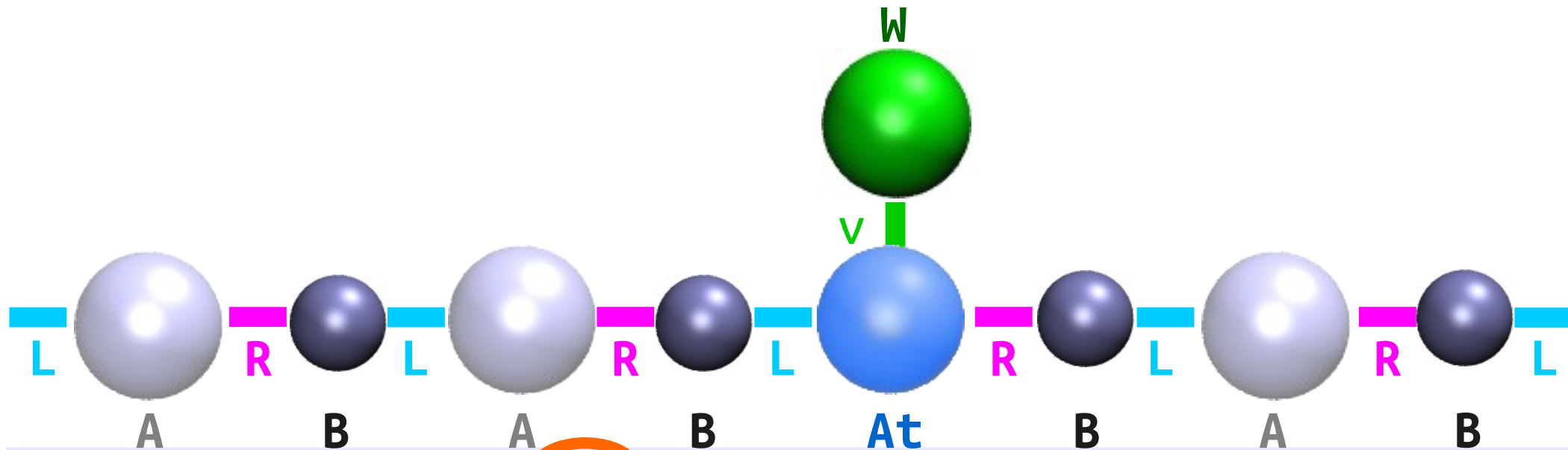
Example: Walking along a polymer
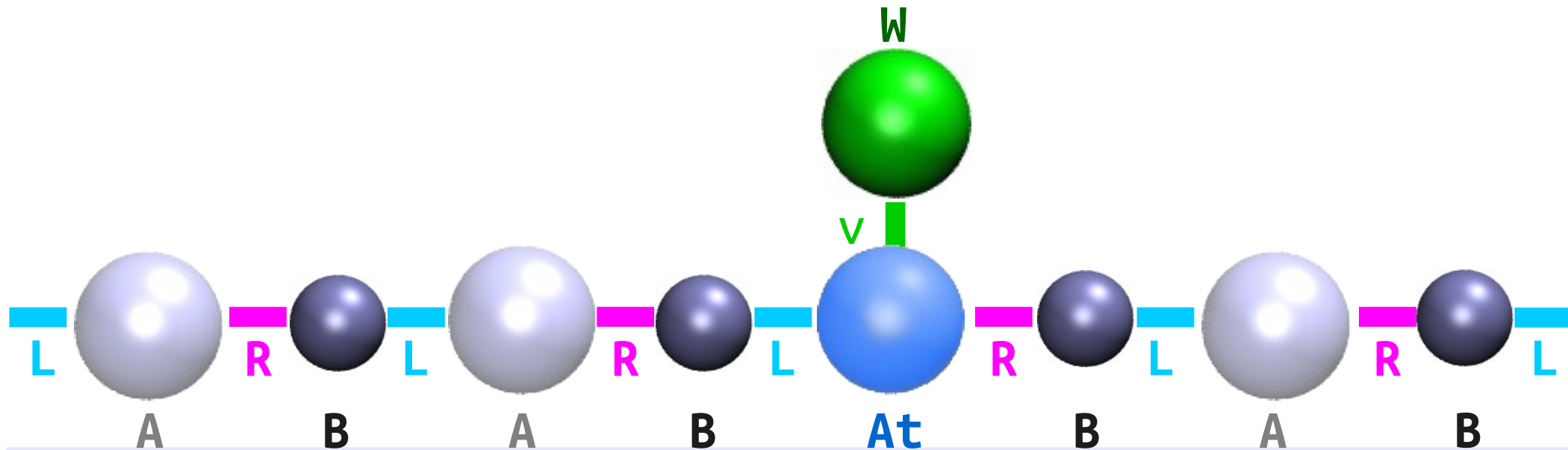


```
fix tr1 all bond/change 100 delay  1
   if atoms @atom:At @atom:B    and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100 delay  2
   if atoms @atom:Bt @atom:A    and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100 delay  3
   if atoms @atom:W  @atom:AT   and  distance <= 1.5
   -> atoms @atom:Wt @atom:At   and  bond @bond:V

fix tr4 all bond/change 100 delay  4
   if atoms @atom:Wt @atom:A    and  bond @bond:V
   -> atoms @atom:W  @atom:A    and  bond BREAK
```
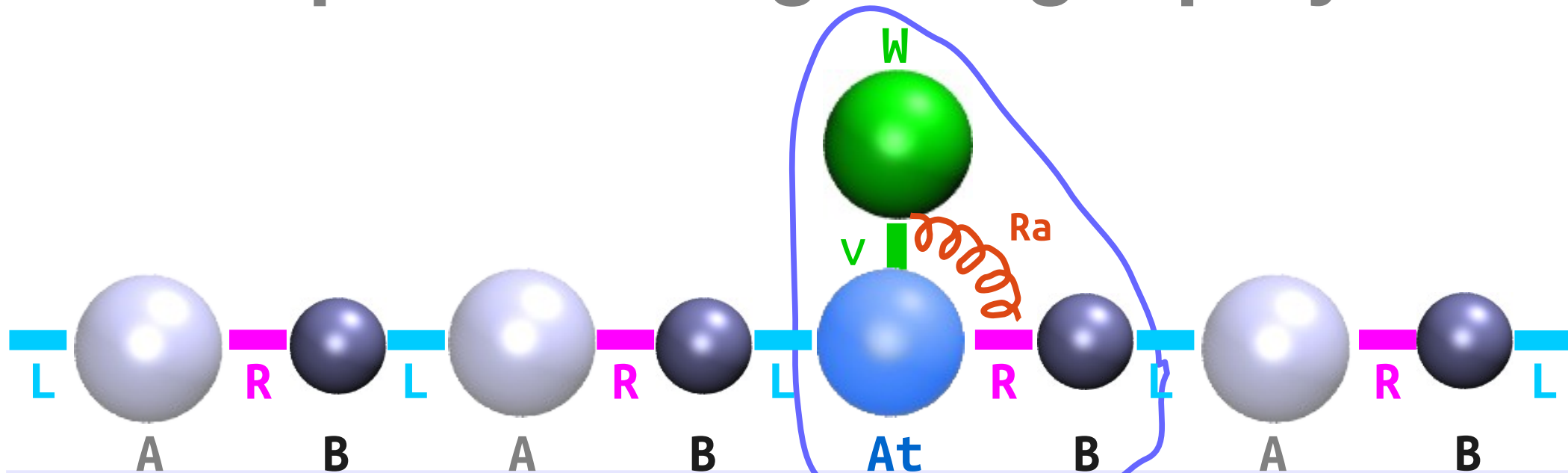
NOW RUN MOLECULAR DYNAMICS
(100 Verlet steps)

(Allow particles to move)

Example: Walking along a polymer
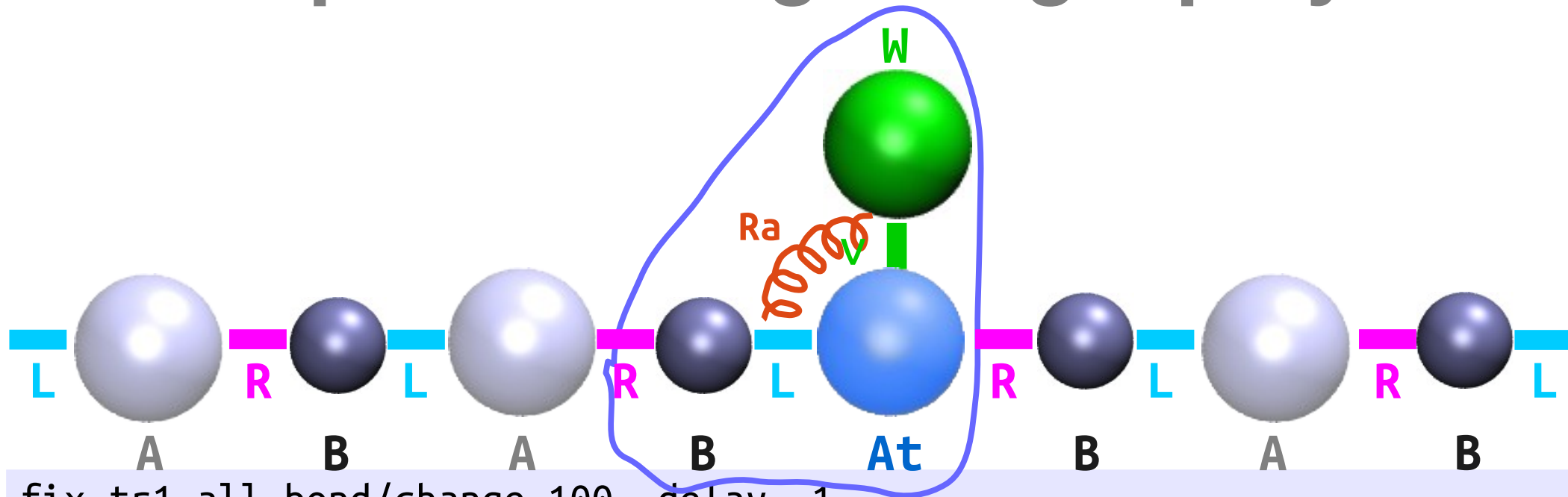


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V

fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```

NOW RUN MOLECULAR DYNAMICS *(100 Verlet steps)*

(Allow particles to move)

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B    and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A    and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT   and  distance <= 1.5
   -> atoms @atom:Wt @atom:At   and  bond @bond:V

fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A    and  bond @bond:V
   -> atoms @atom:W  @atom:A    and  bond BREAK
```

NOW RUN MOLECULAR DYNAMICS *(100 Verlet steps)*
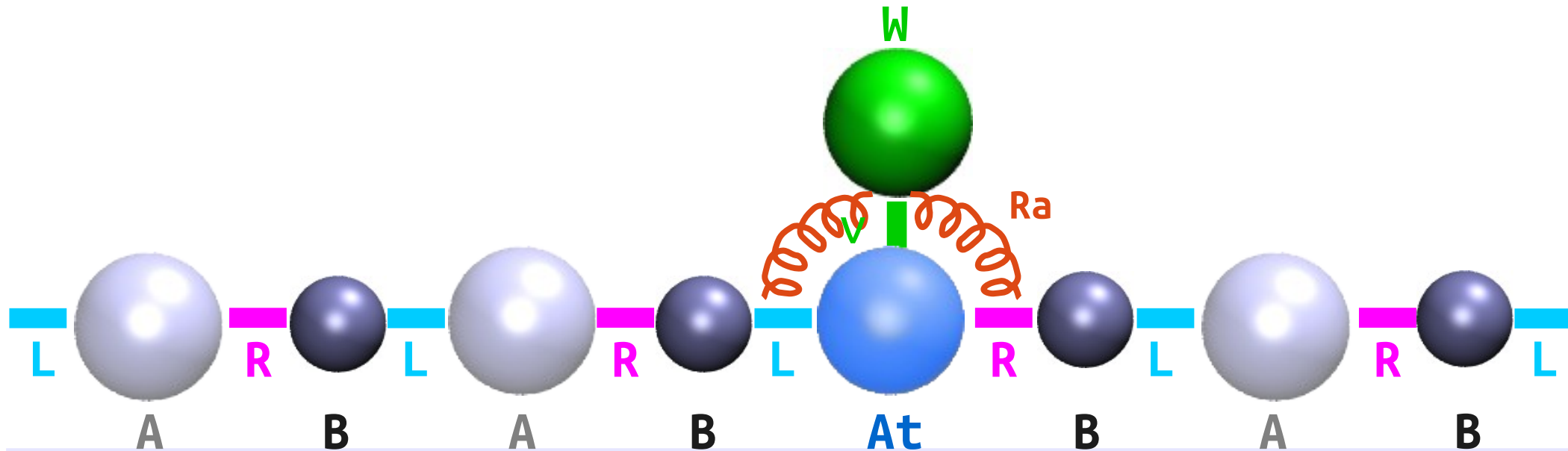
(Allow particles to move)

Example: Walking along a polymer
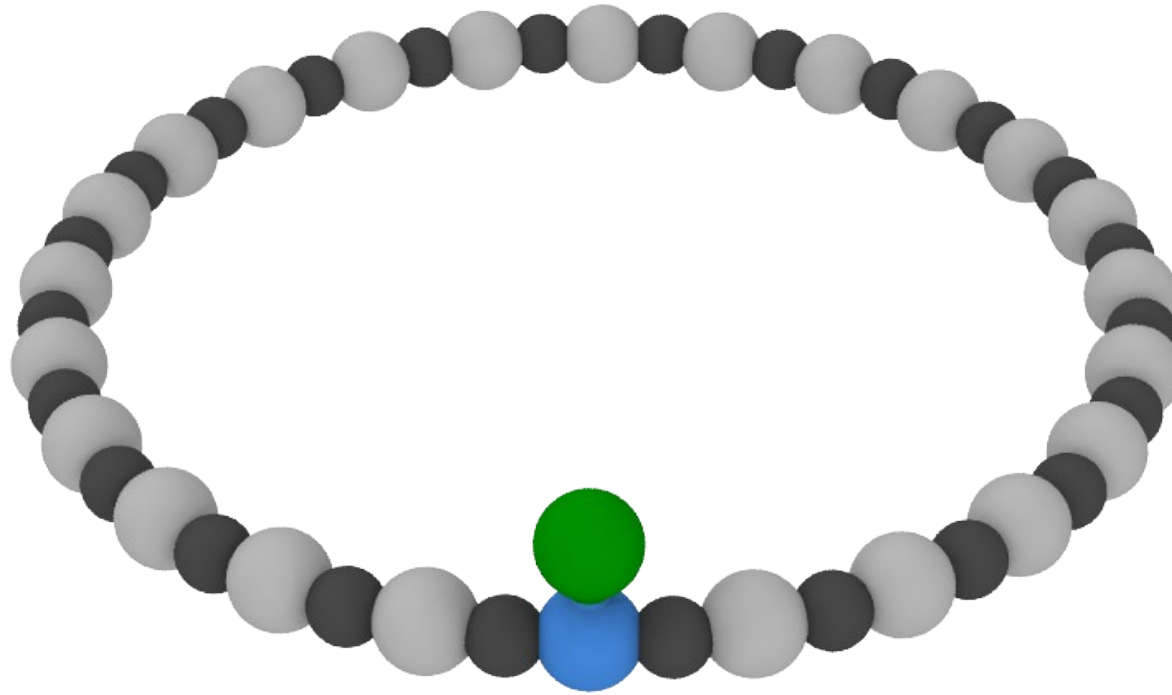


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V
       and angle @angle:Ra  @atom:B @atom:At @atom:W
fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new     100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V
      and angle @angle:Ra  @atom:B @atom:At @atom:W
fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```
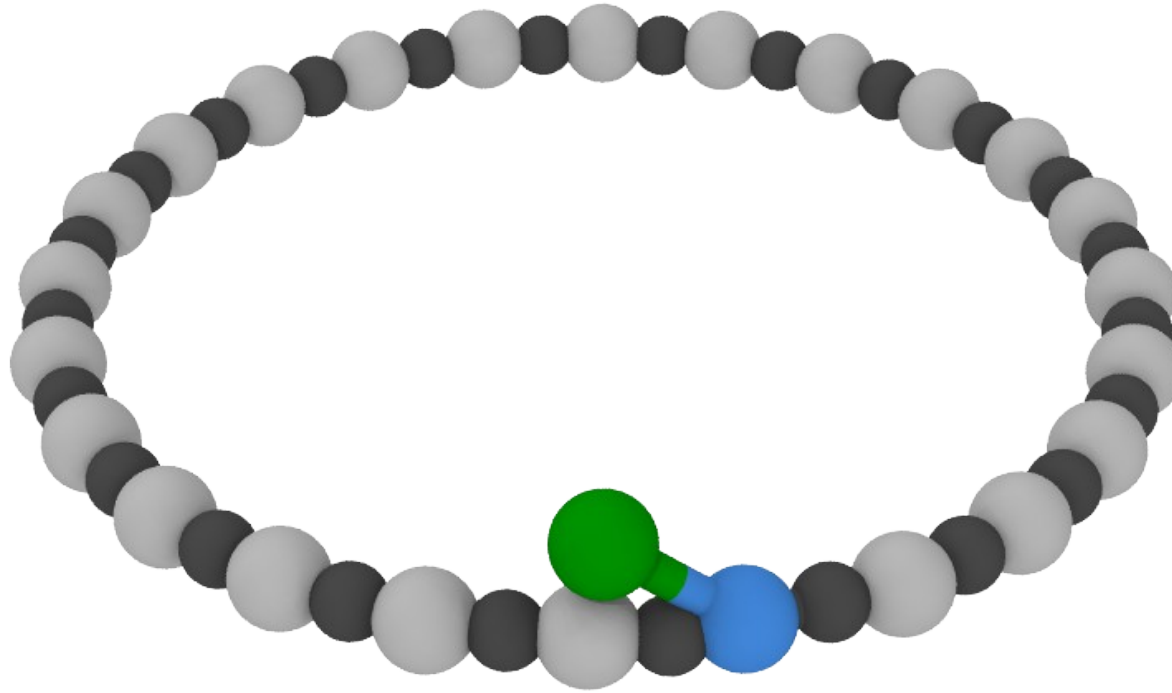
Example: Walking along a polymer
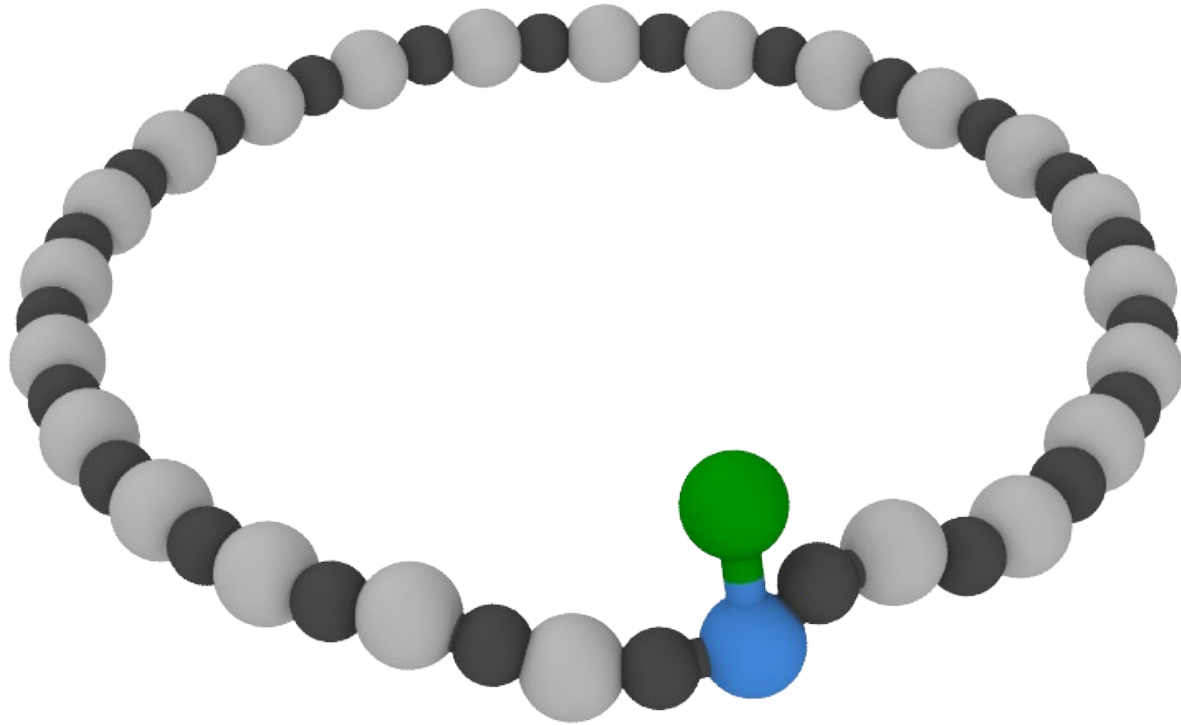


```
fix tr1 all bond/change 100   delay  1
    if atoms @atom:At @atom:B    and   bond @bond:R   and   prob 0.2
    -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100   delay  2
    if atoms @atom:Bt @atom:A    and   bond @bond:L
    -> atoms @atom:B  @atom:AT
fix tr3 all bond/new     100   delay  3
    if atoms @atom:W  @atom:AT   and   distance <= 1.5
    -> atoms @atom:Wt @atom:At   and   bond @bond:V
       and  angle @angle:Ra   @atom:B @atom:At @atom:W
fix tr4 all bond/change 100   delay  4
    if atoms @atom:Wt @atom:A    and   bond @bond:V
    -> atoms @atom:W  @atom:A    and   bond BREAK
```

Example: Walking along a polymer


```
fix tr1 all bond/change 100  delay  1
   if atoms @atom:At @atom:B   and  bond @bond:R  and  prob 0.2
   -> atoms @atom:A  @atom:Bt
fix tr2 all bond/change 100  delay  2
   if atoms @atom:Bt @atom:A   and  bond @bond:L
   -> atoms @atom:B  @atom:AT
fix tr3 all bond/new    100  delay  3
   if atoms @atom:W  @atom:AT  and  distance <= 1.5
   -> atoms @atom:Wt @atom:At  and  bond @bond:V
      and angle @angle:Ra  @atom:B @atom:At @atom:W
fix tr4 all bond/change 100  delay  4
   if atoms @atom:Wt @atom:A   and  bond @bond:V
   -> atoms @atom:W  @atom:A   and  bond BREAK
```

Example: Walking along a polymer

Example: Walking along a polymer

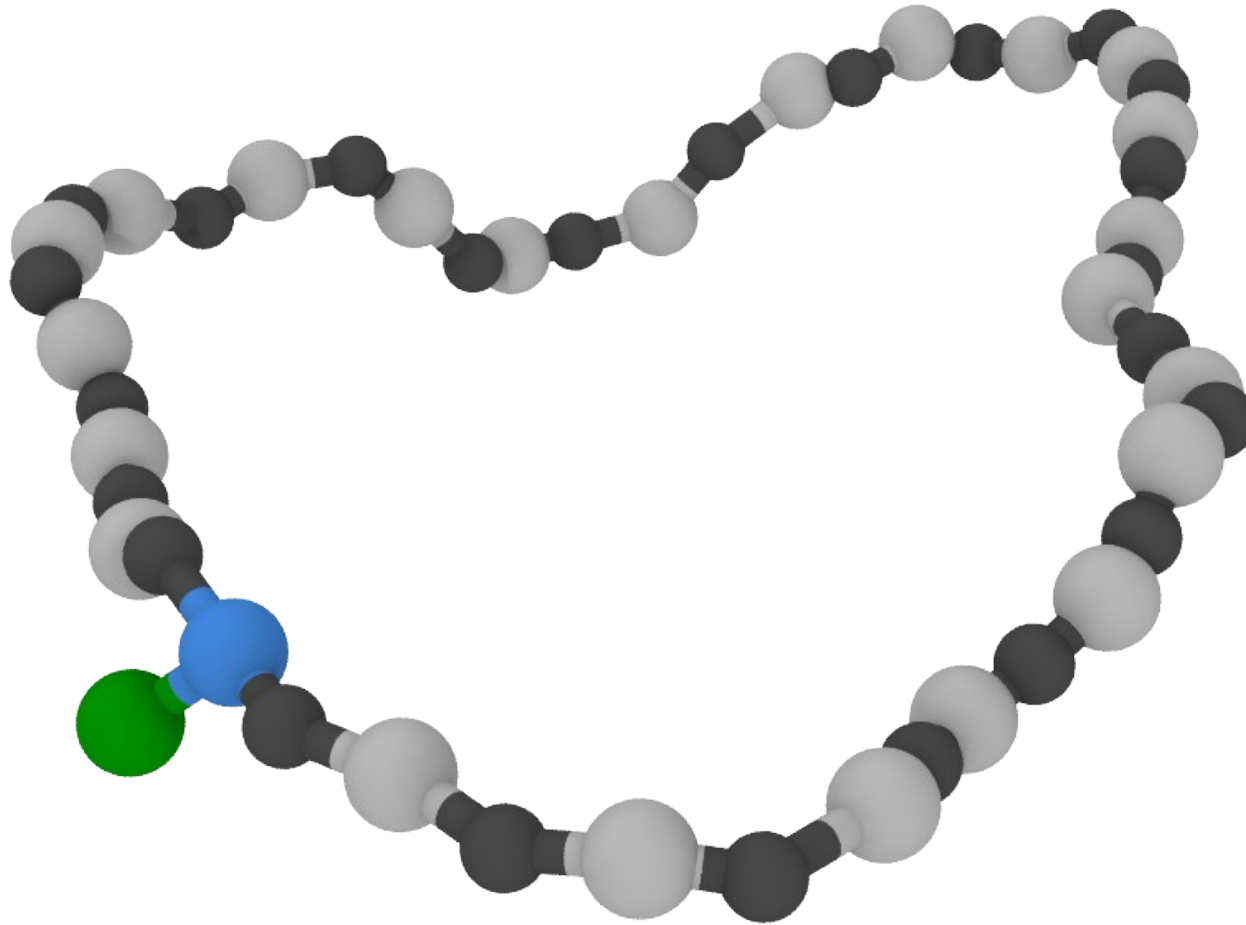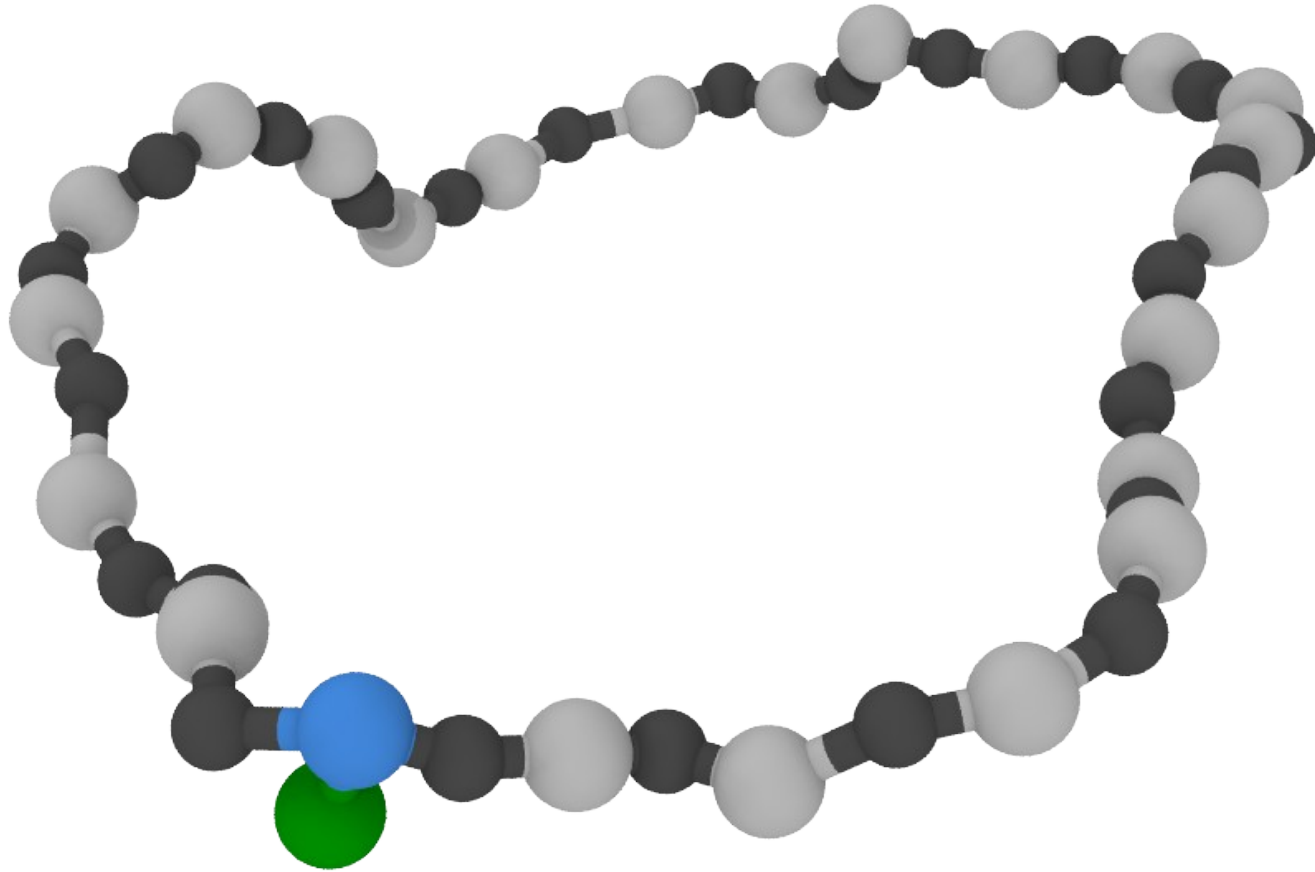# Example: Walking along a polymer

Example: Walking along a polymer

Example: Walking along a polymer

Example: Walking along a polymer

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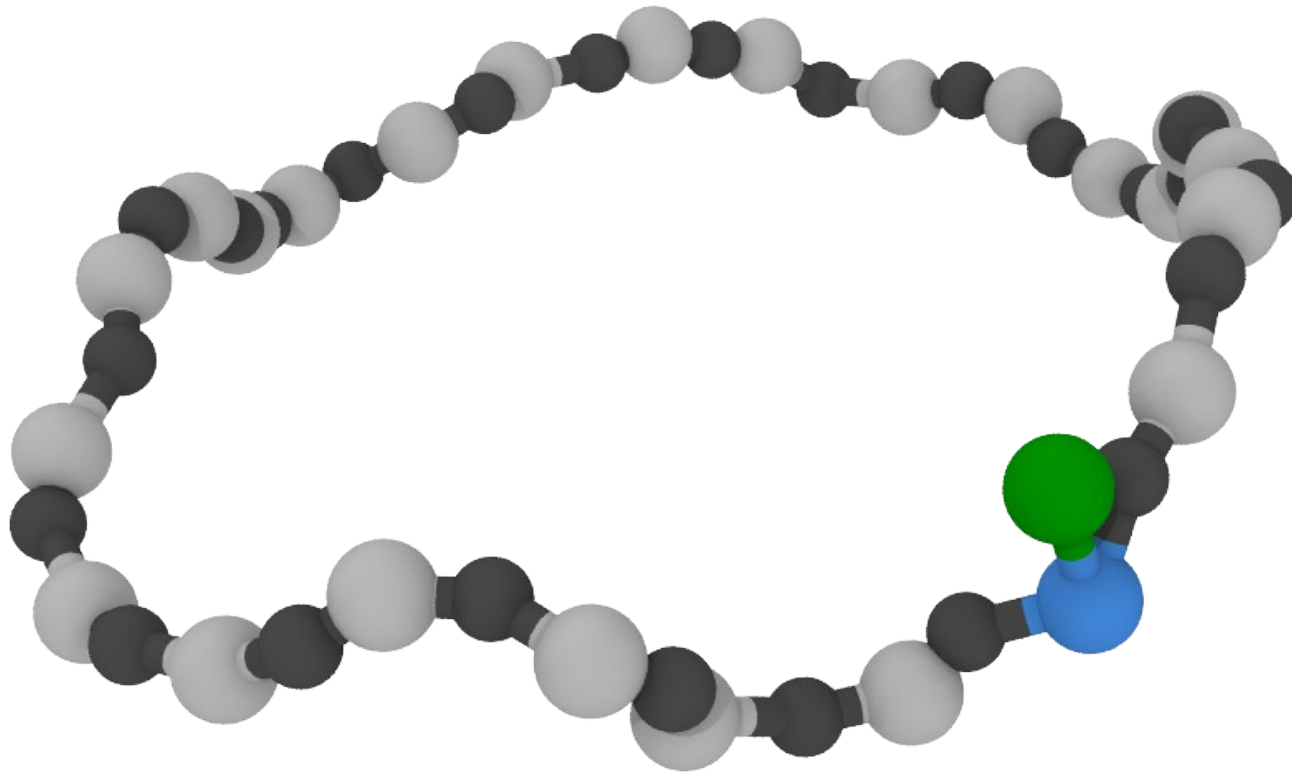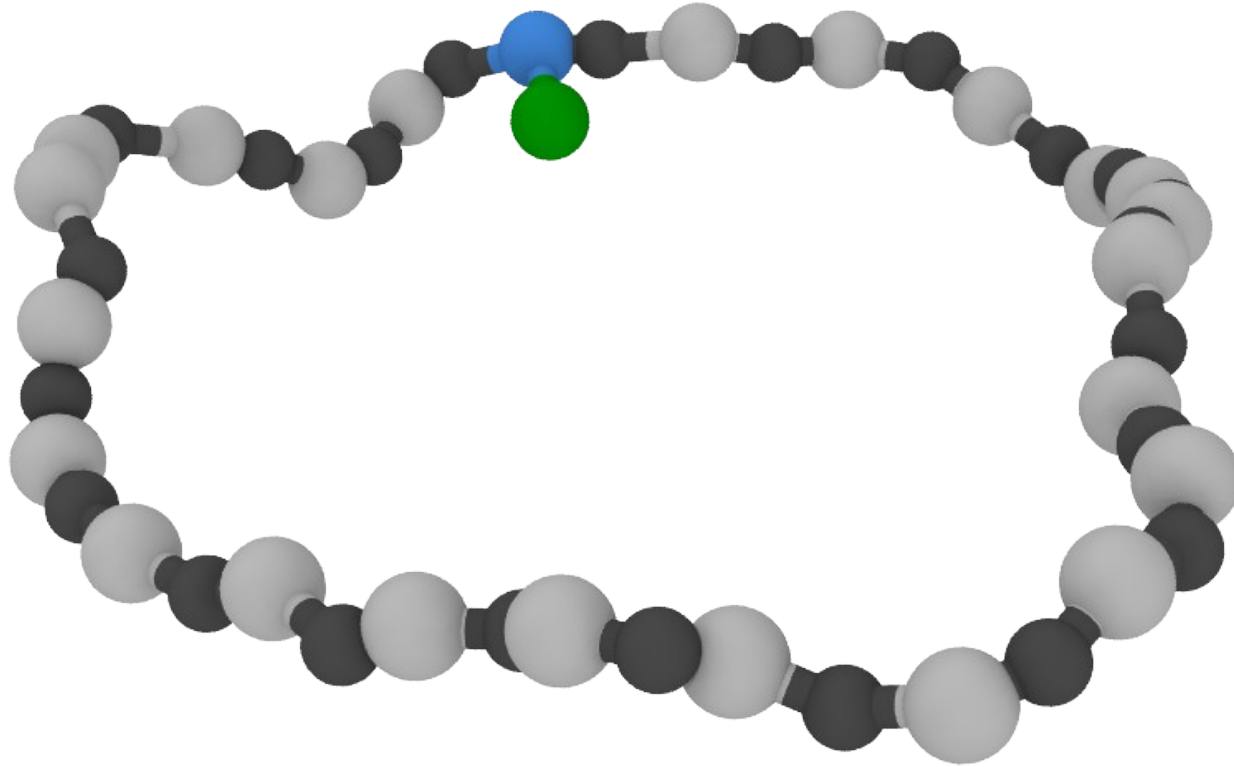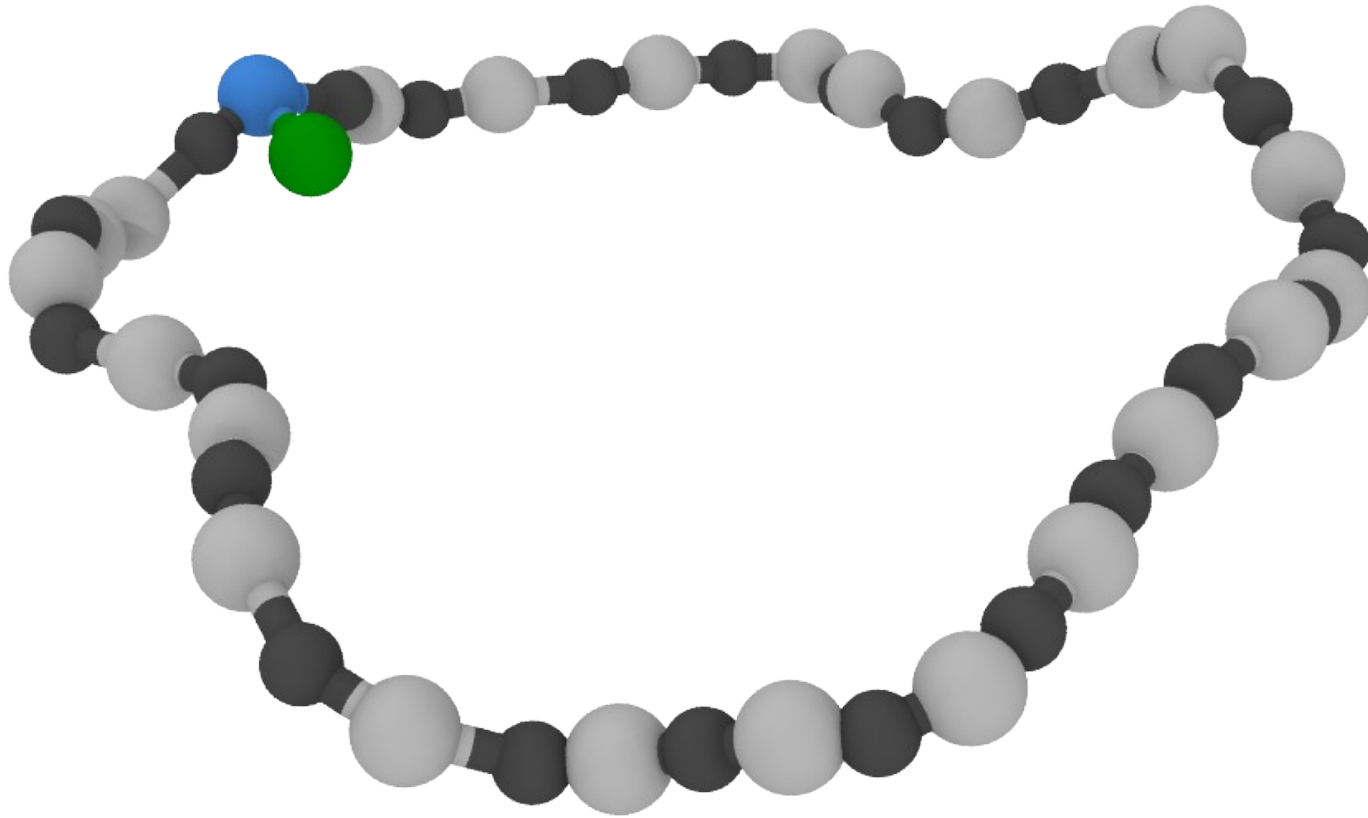# Example: Walking along a polymer

Example: Walking along a polymer

Example: Walking along a polymer

Example: Walking along a polymer

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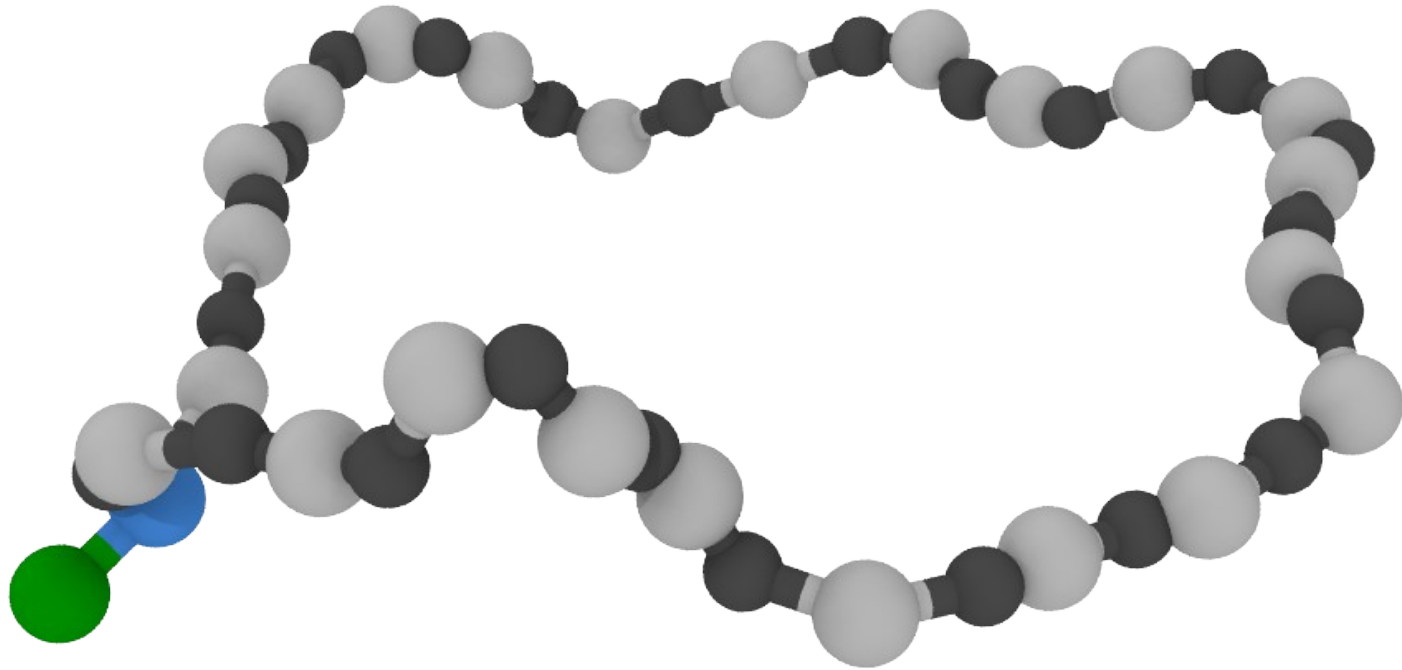# Example: Walking along a polymer

Example: Walking along a polymer

Example: Walking along a polymer

Example: Walking along a polymer

Example: Walking along a polymer

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Example: Walking along a polymer