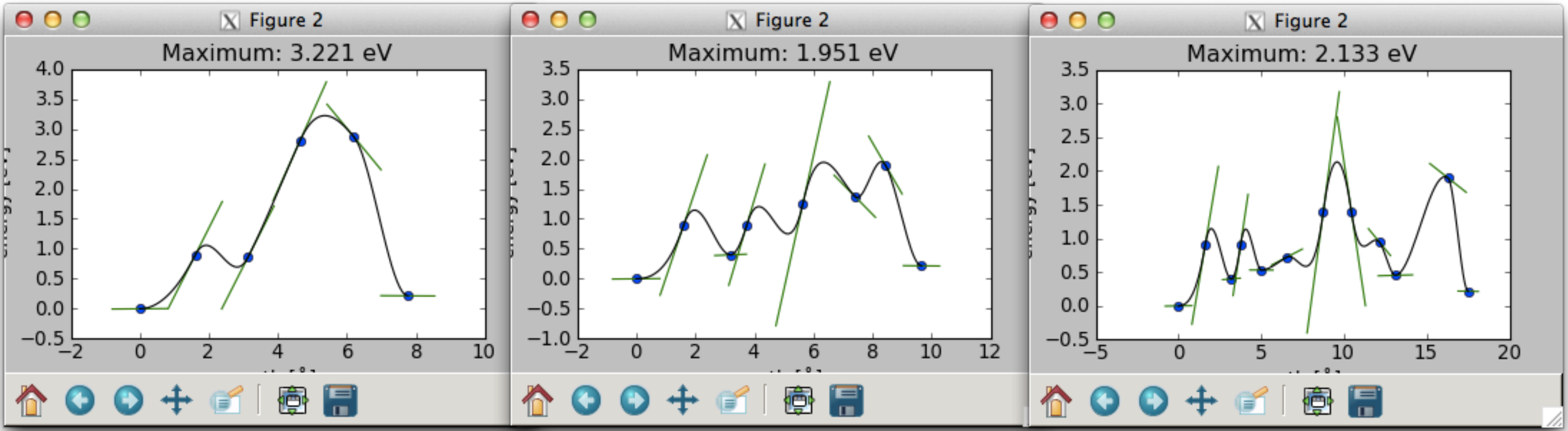
# Challenges with the currently (correctly) implemented NEB-method. Should ASE revert to the original more robust NEB-formulation with springs?

Bjørk Hammer
Aarhus University, Denmark

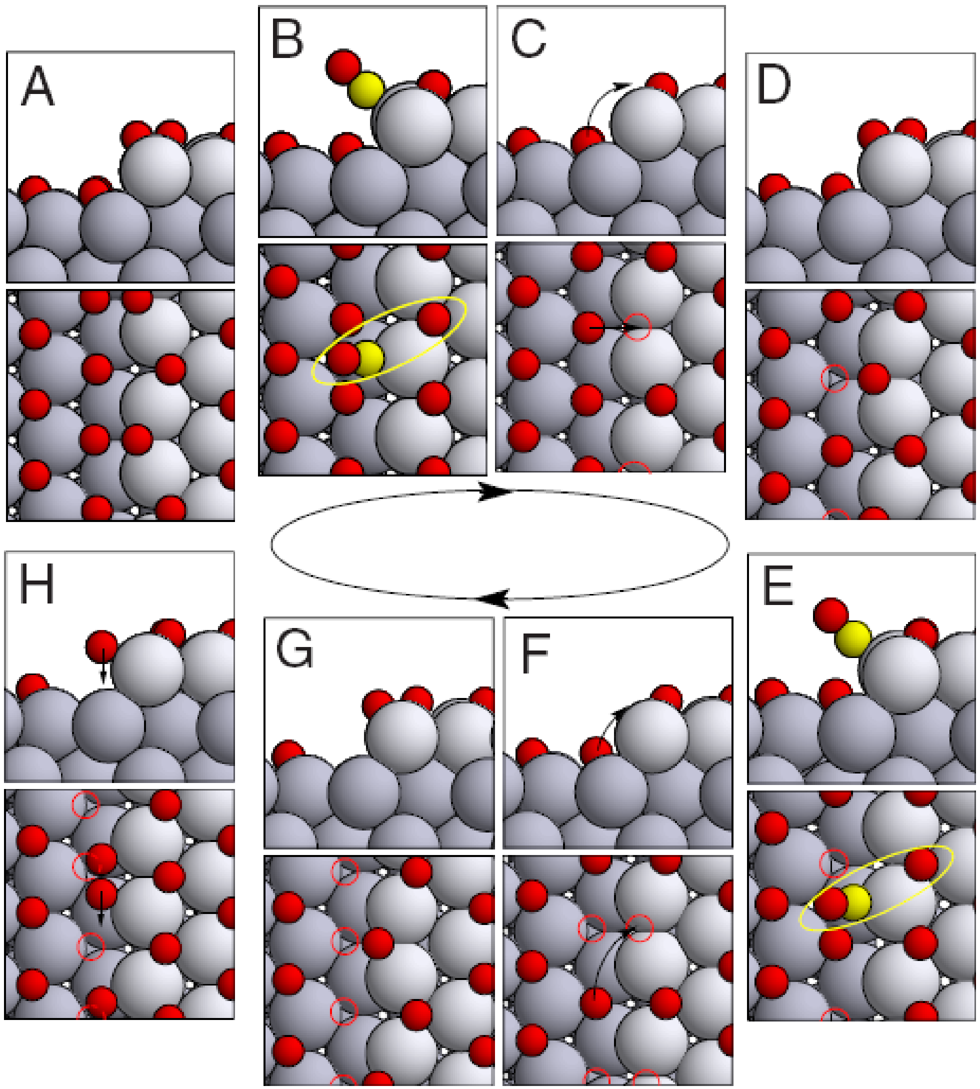
- **Motivation:** often seen that finding saddle points with ASE is challenging.
- **Objective:** assure easy and simple access to saddle point search with ASE
- **Means:**
  - Illustrate pit-falls of current NEB implementation
  - Illustrate robustness of old NEB implementation

# Challenges with the currently (correctly)

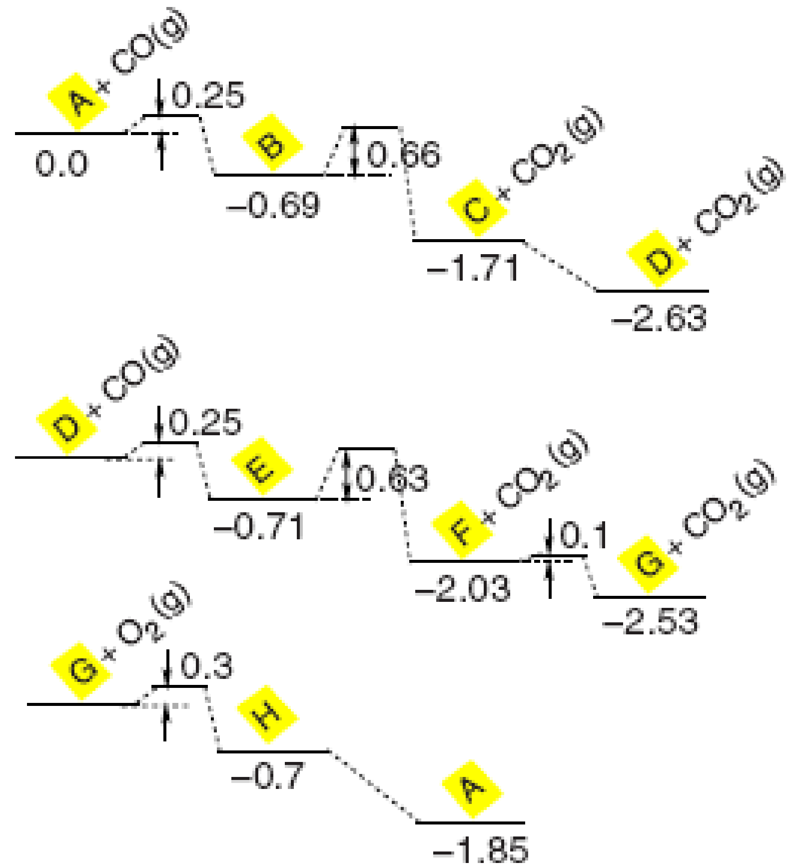



- **Motivation:** often seen that finding saddle points with ASE is challenging.
- **Objective:** assure easy and simple access to saddle point search with ASE
- **Means:**
  - Illustrate pit-falls of current NEB implementation
  - Illustrate robustness of old NEB implementation

# Activity of fully oxygen covered stepped metal surfaces

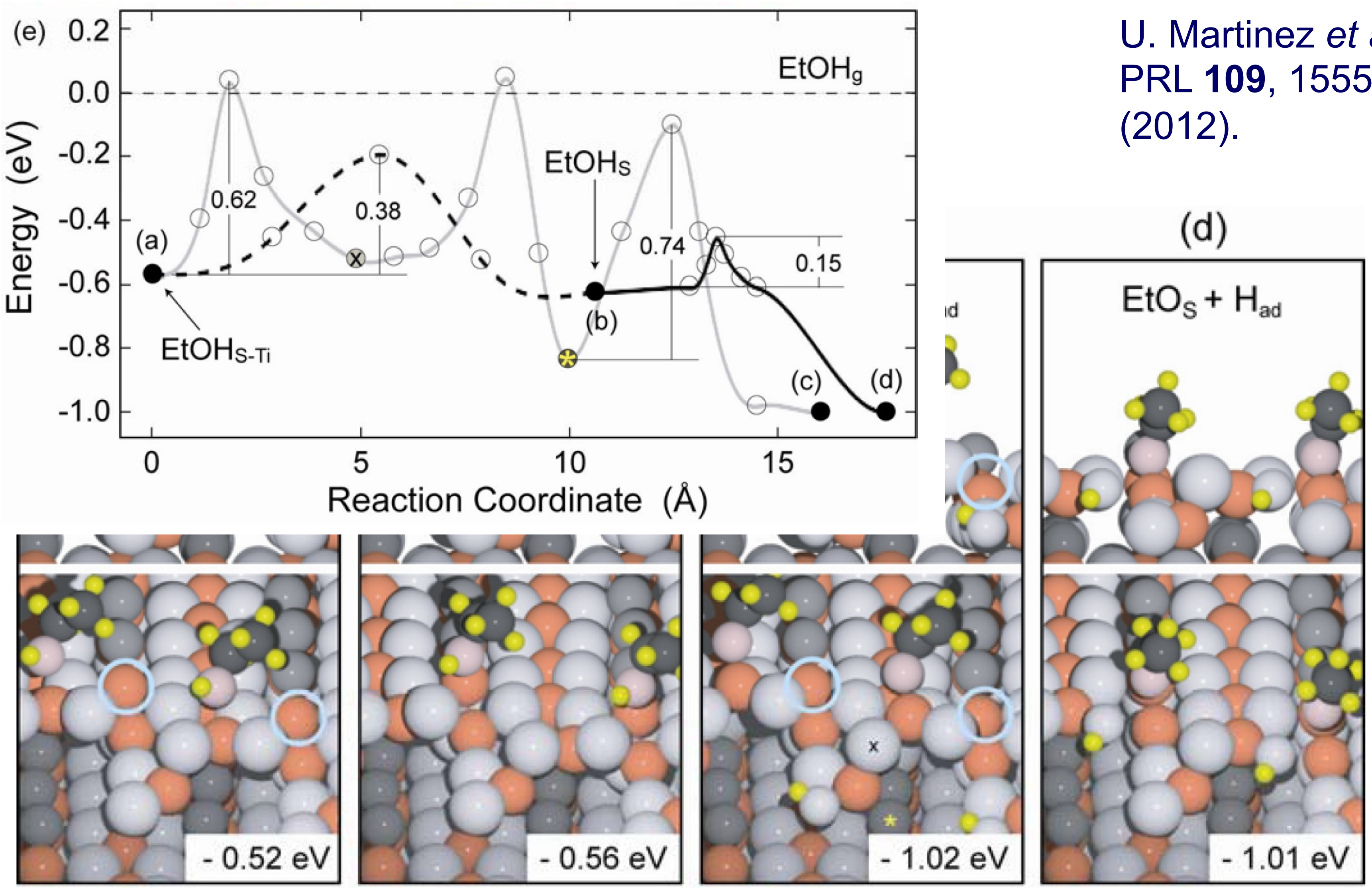



Z. Sljivancanin and BH,
Phys Rev B 81, 121413(R) (2010)

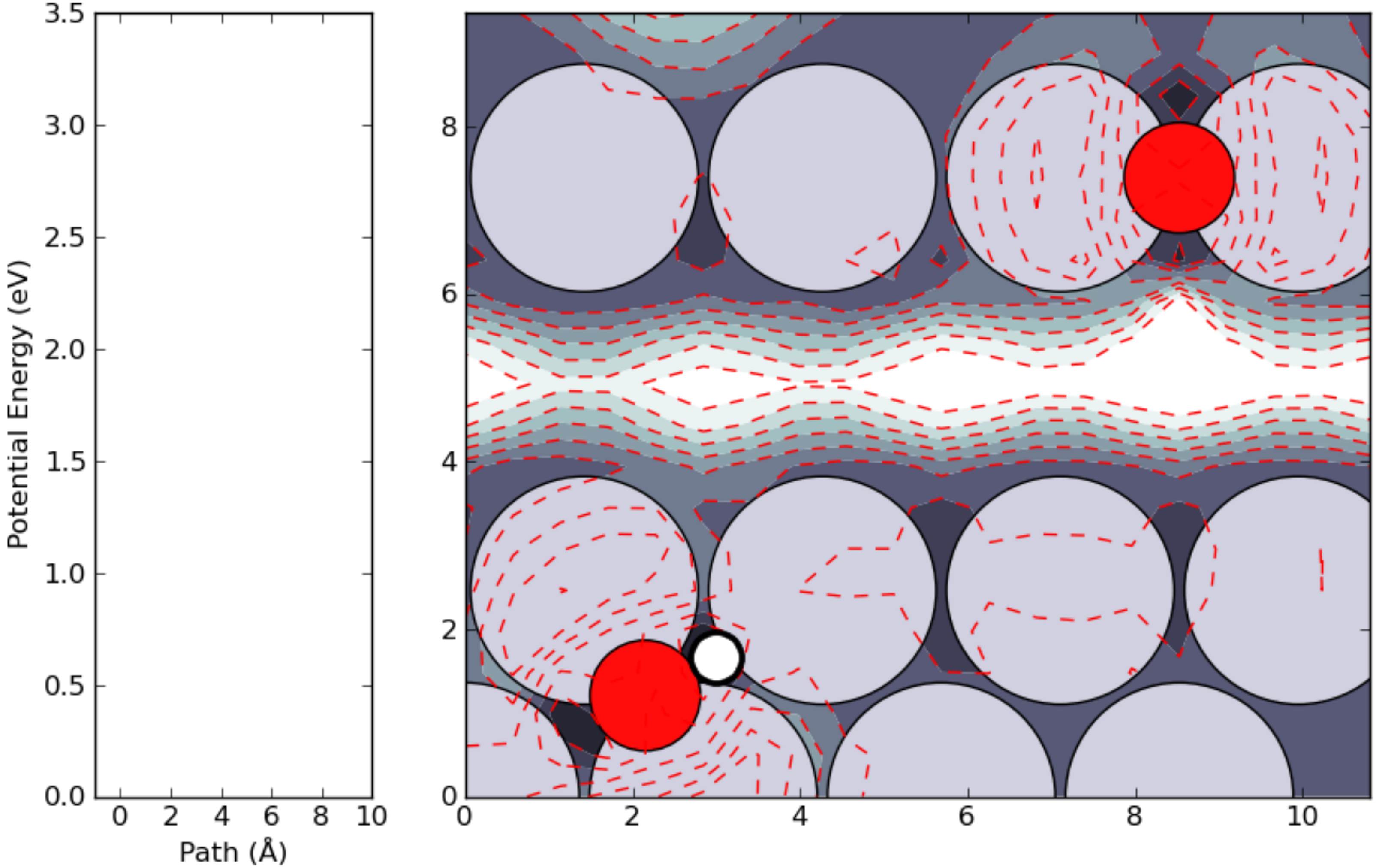


# Ethanol dissociation

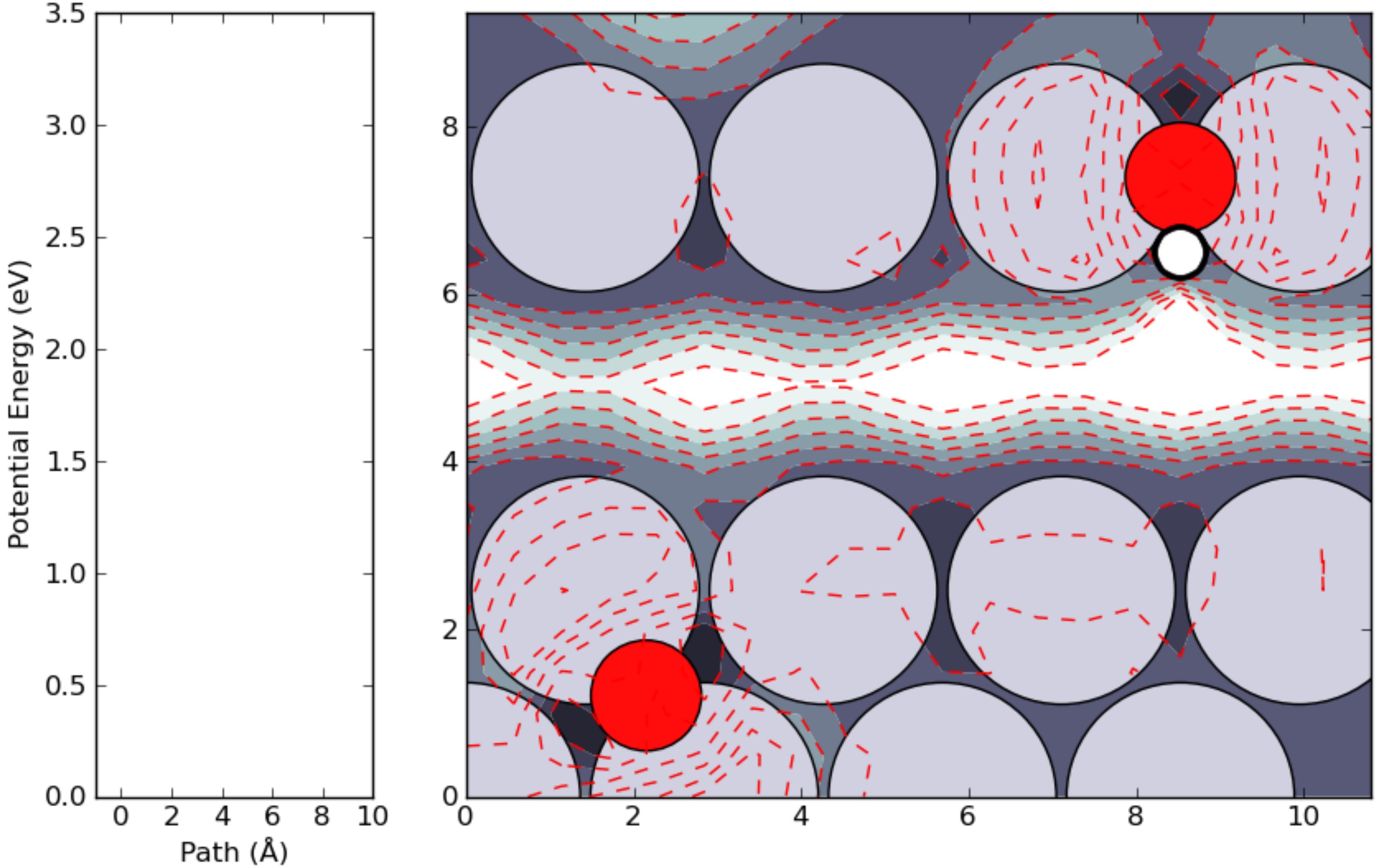
U. Martinez *et al.*, PRL **109**, 155501 (2012).



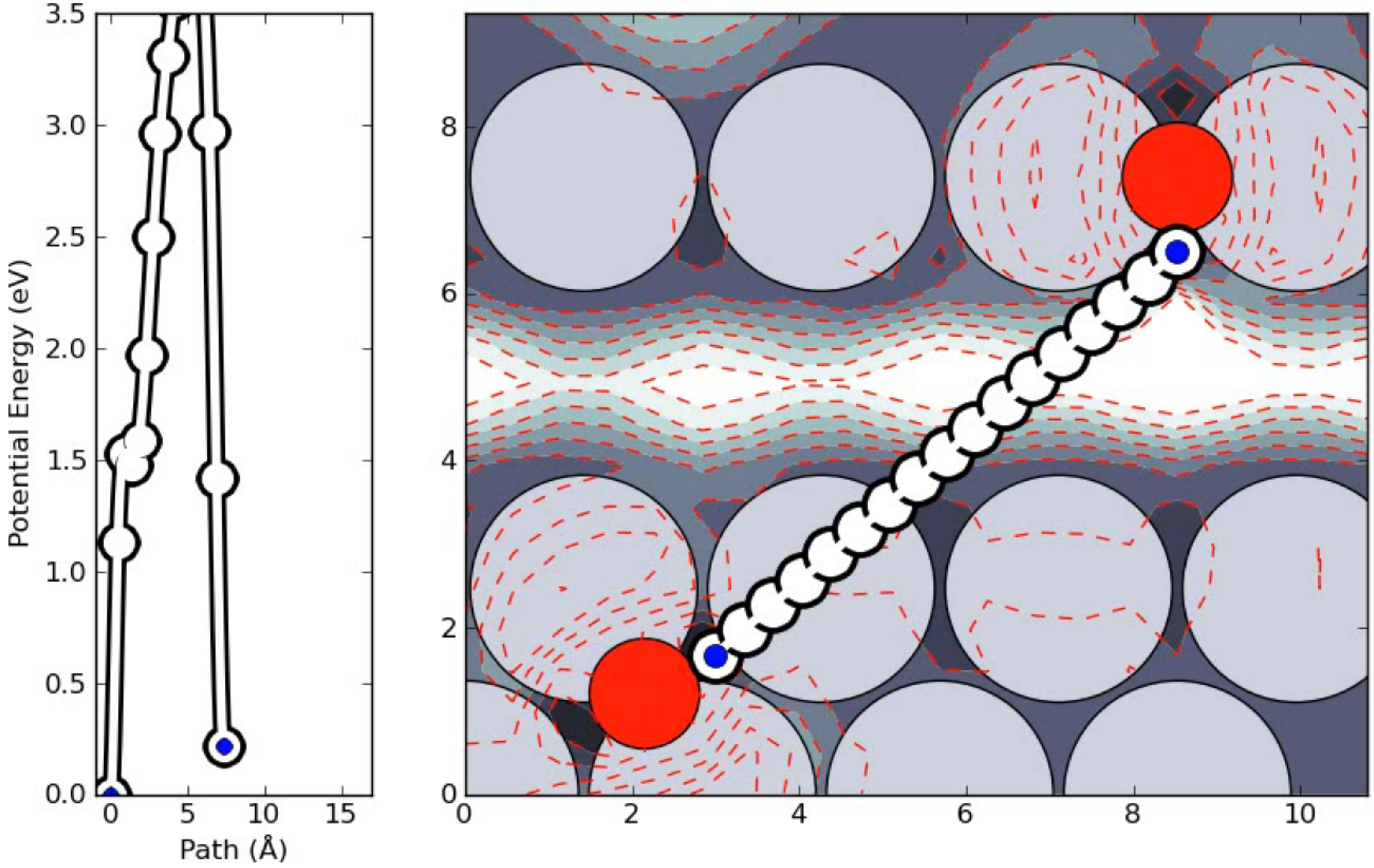
# Model system: Initial configuration



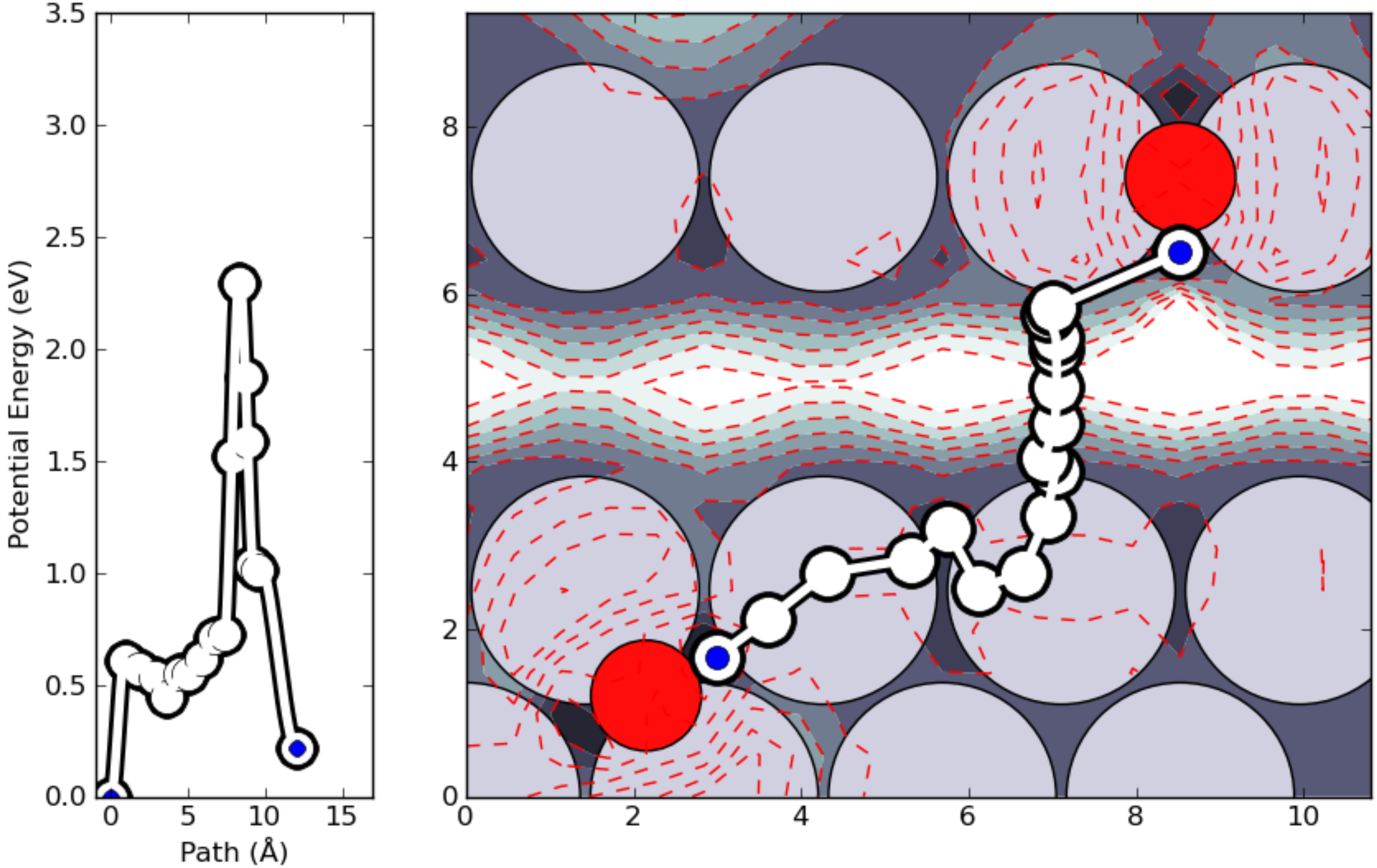
# Model system: Final configuration



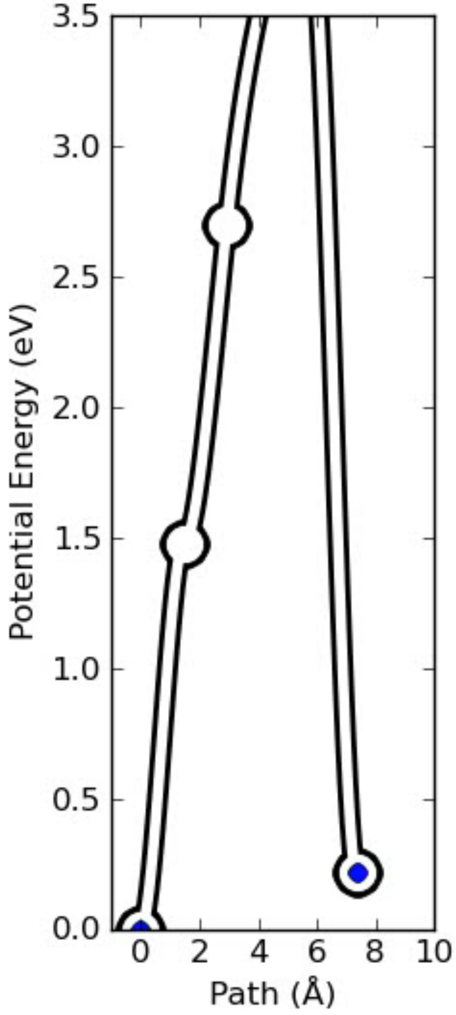
# Success 1: Linear interpolation, many images

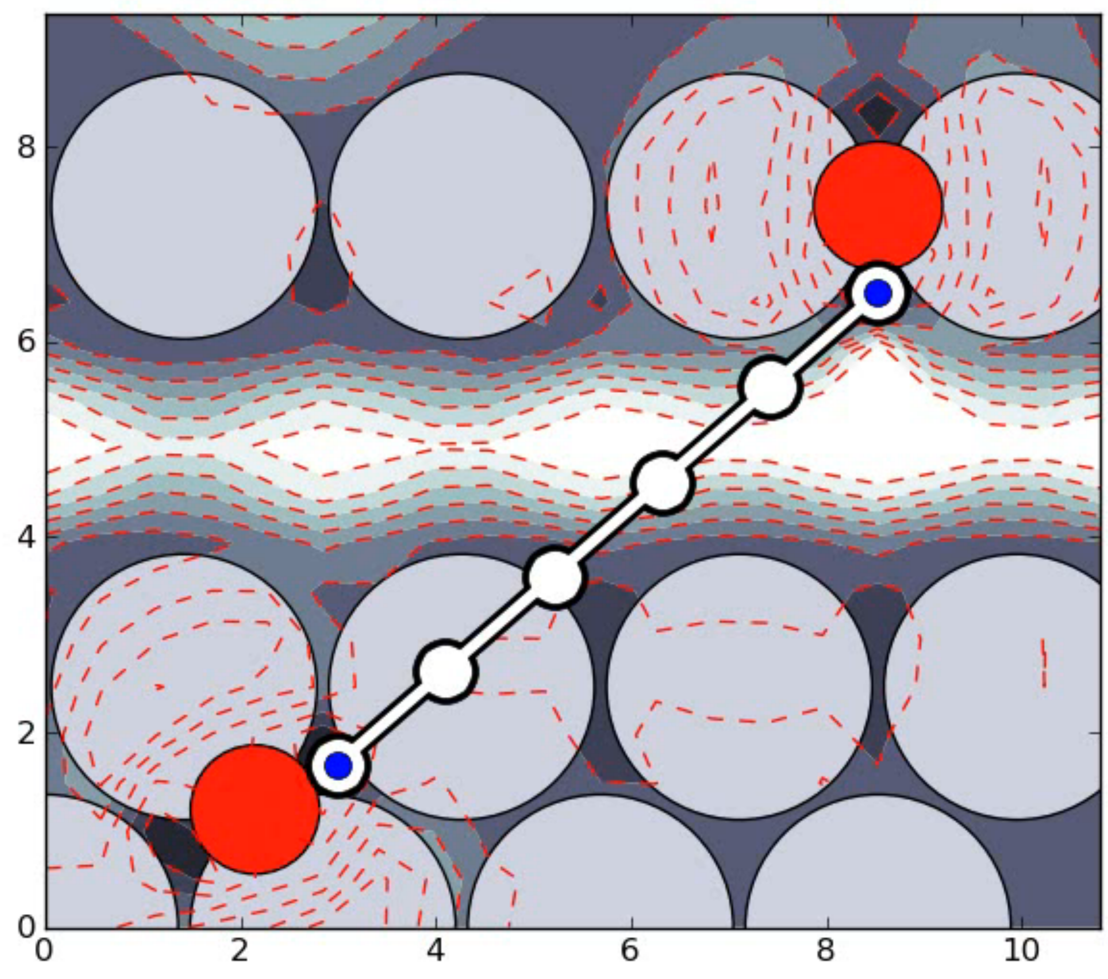


# Success 1: standard ASE-NEB, many images

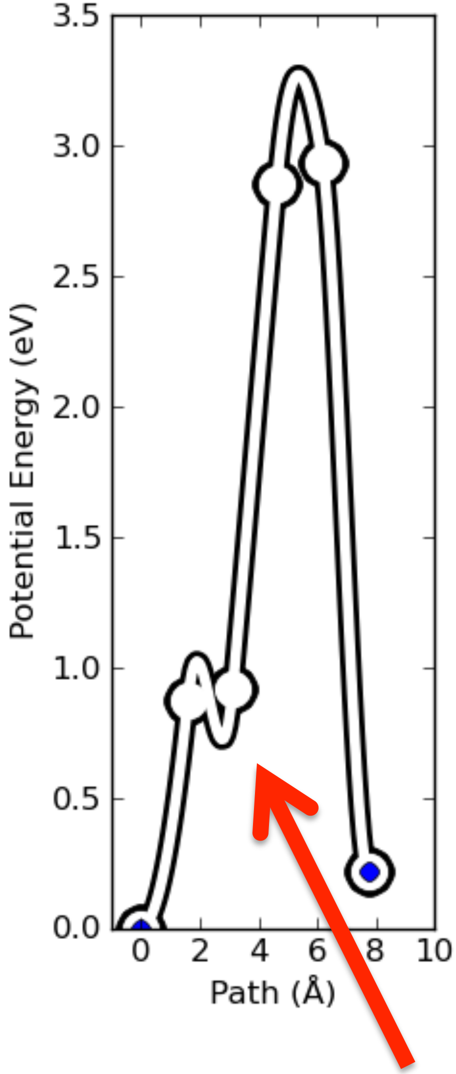


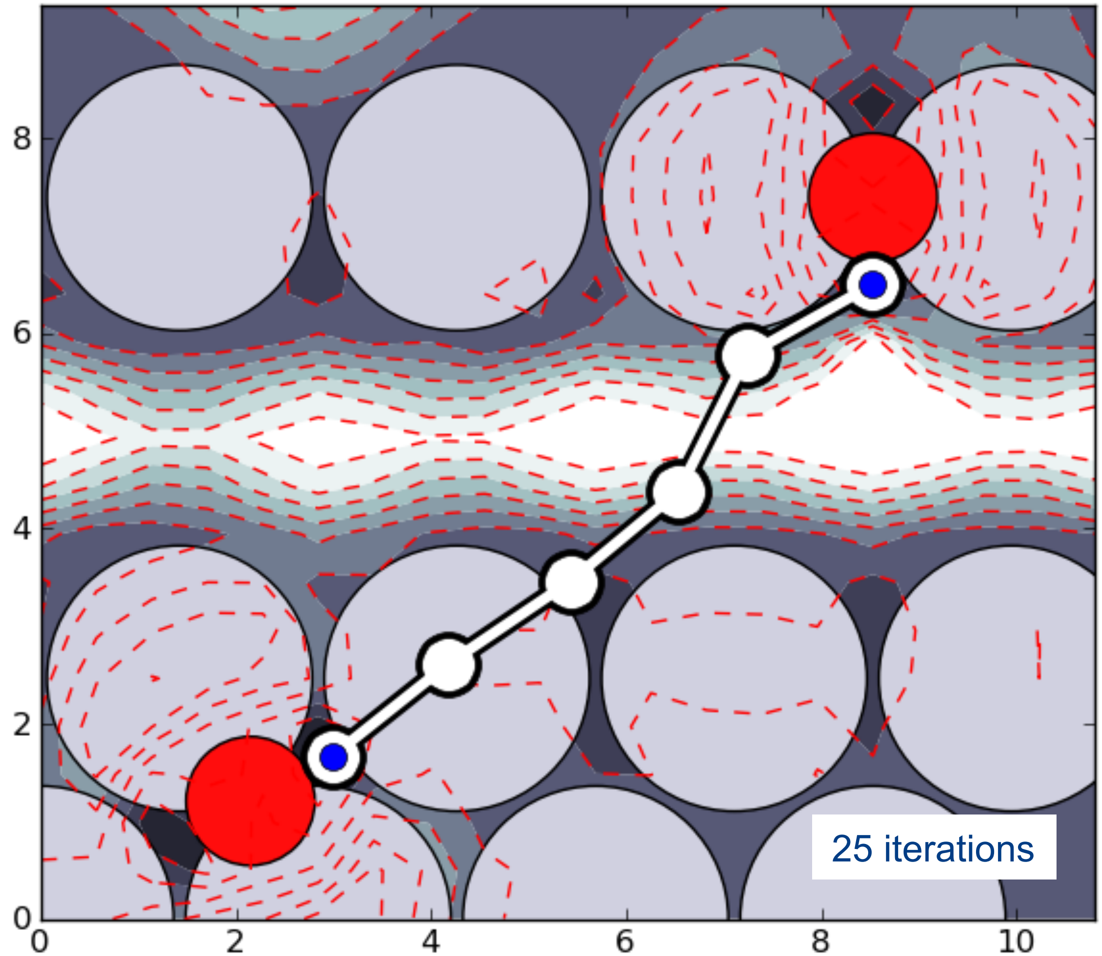
# More typical: Few images.



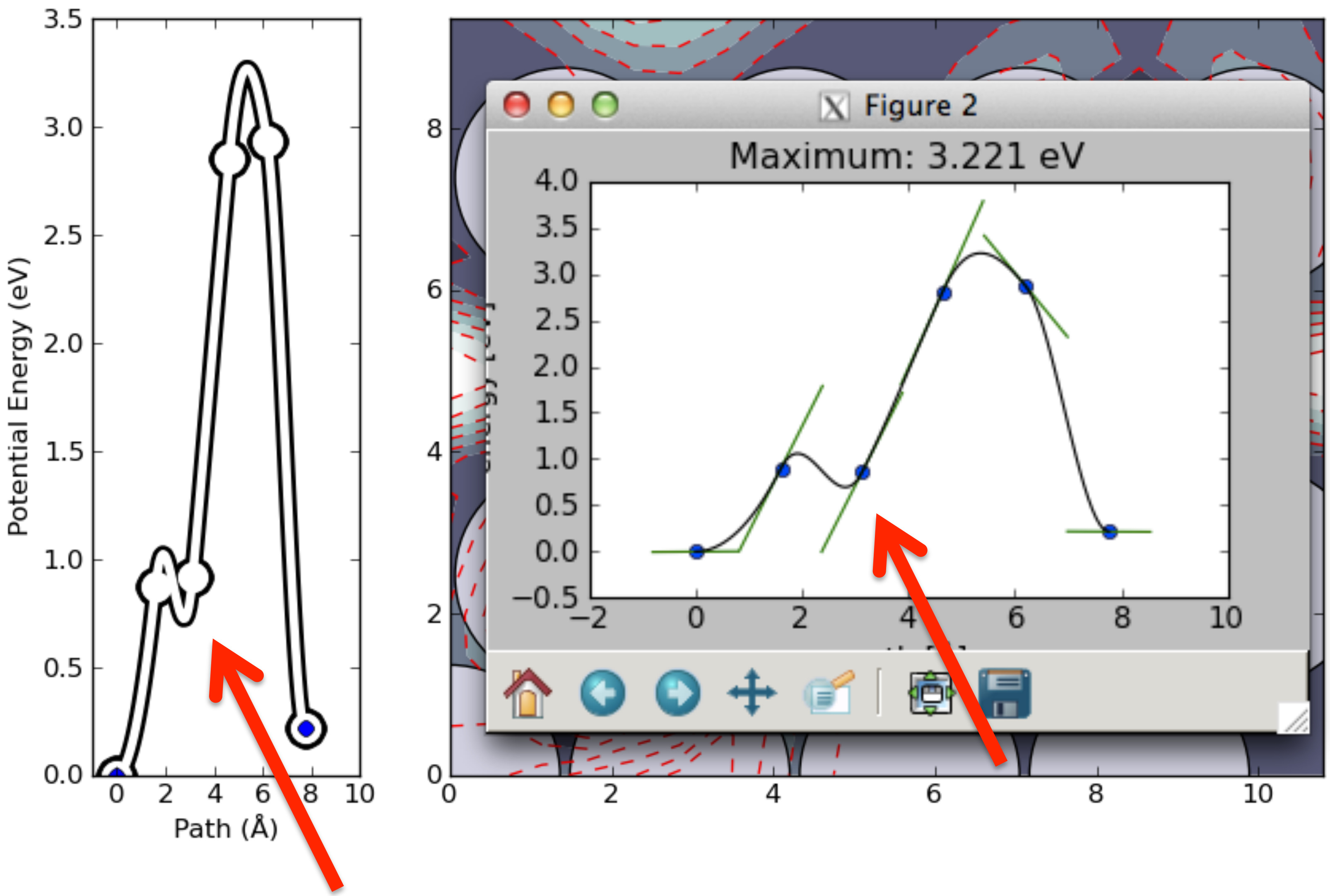



# After some iterations: a local minimum

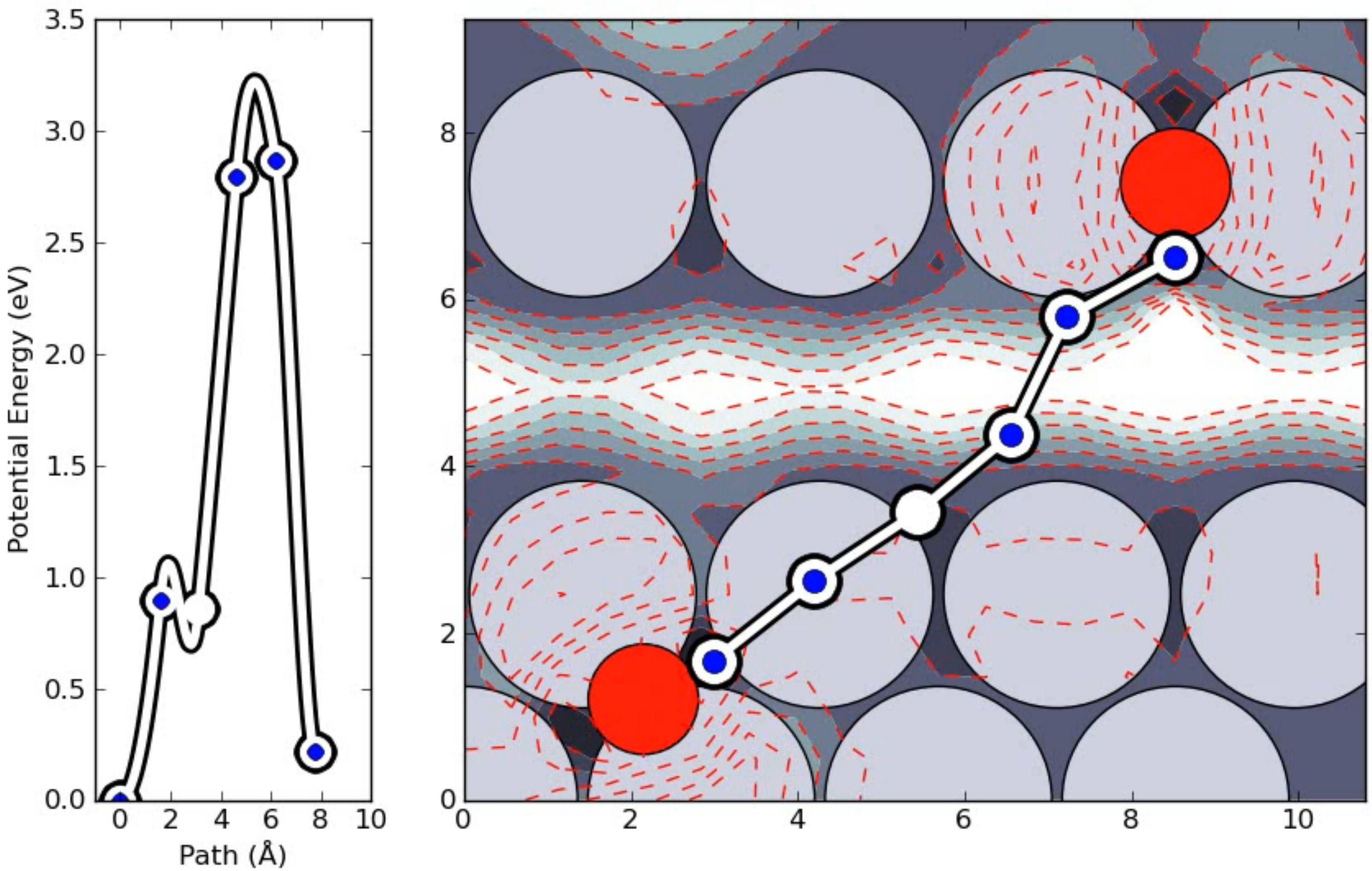


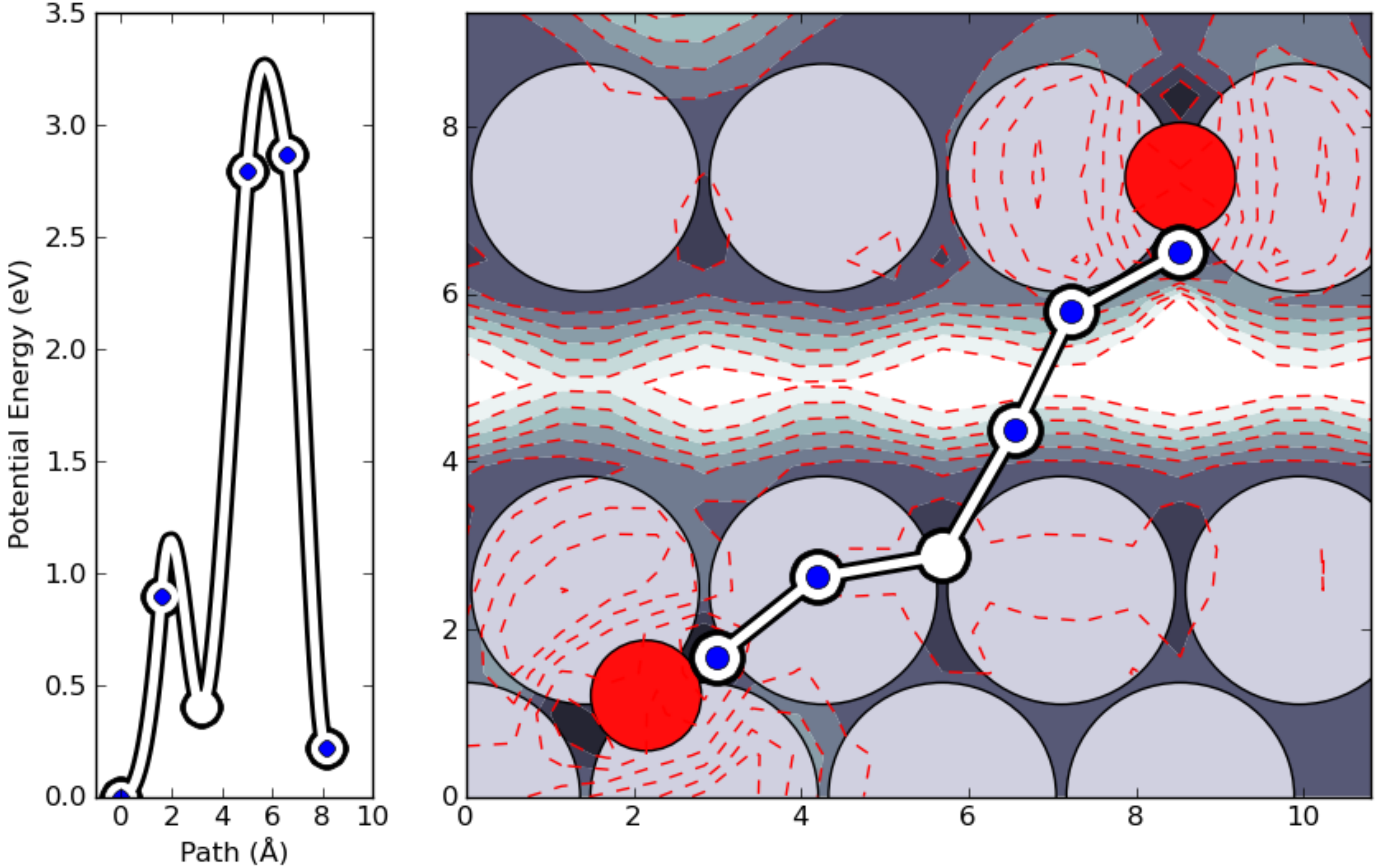
# After some iterations: a local minimum



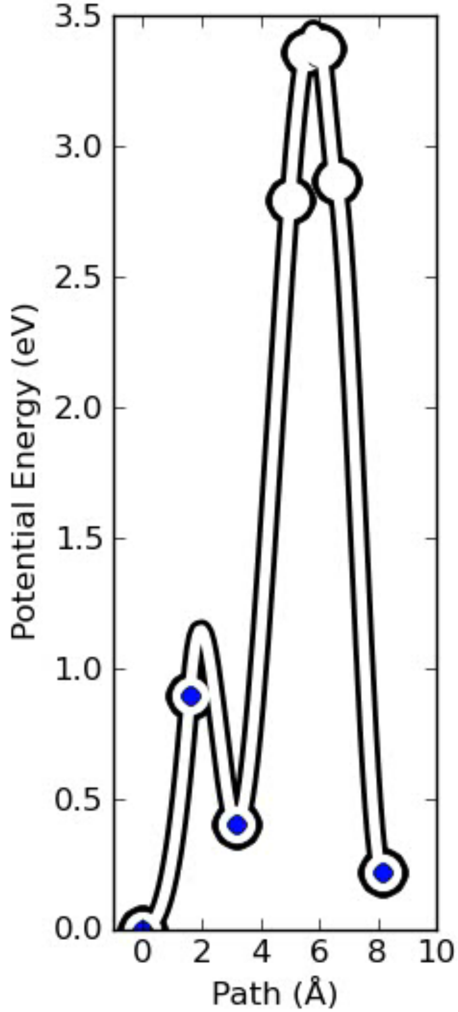
# Identifying the local minimum along the path

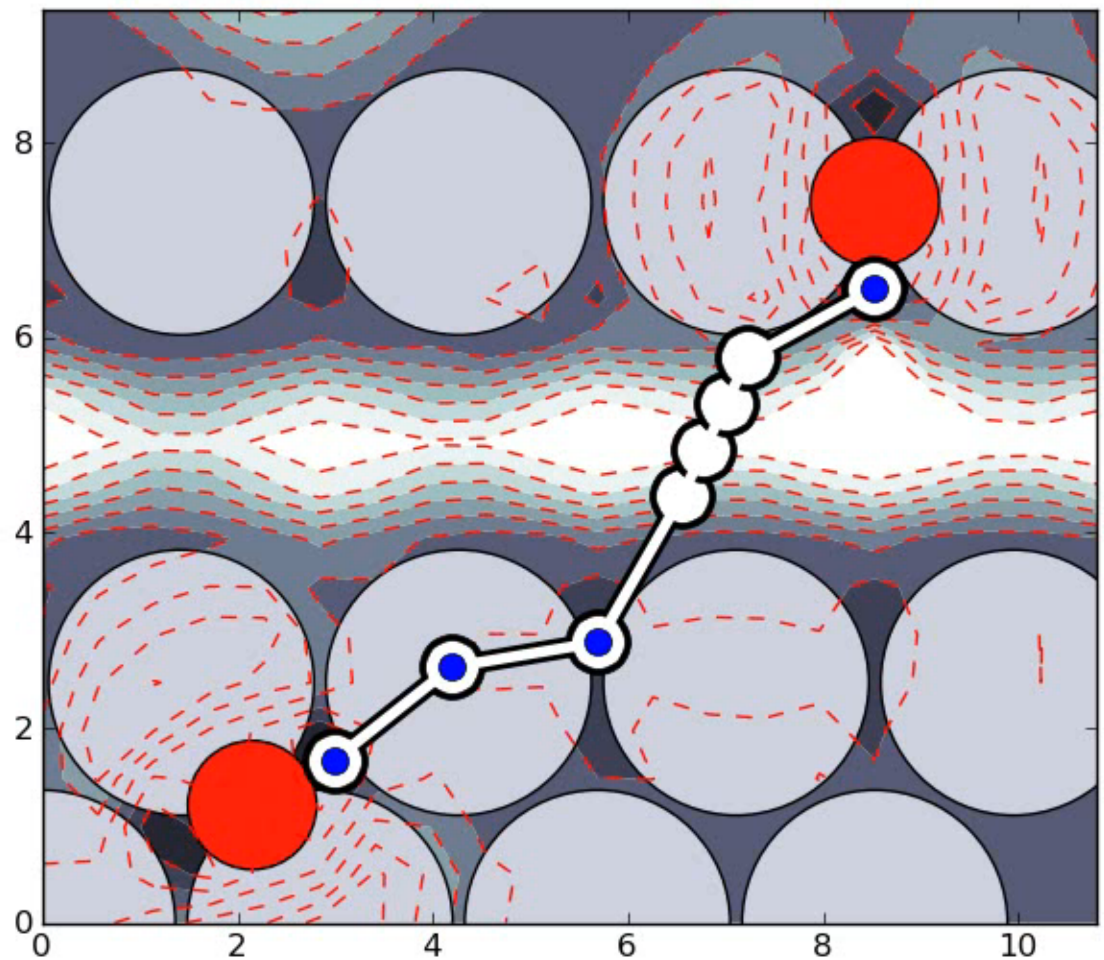


# Identifying the local minimum along the path

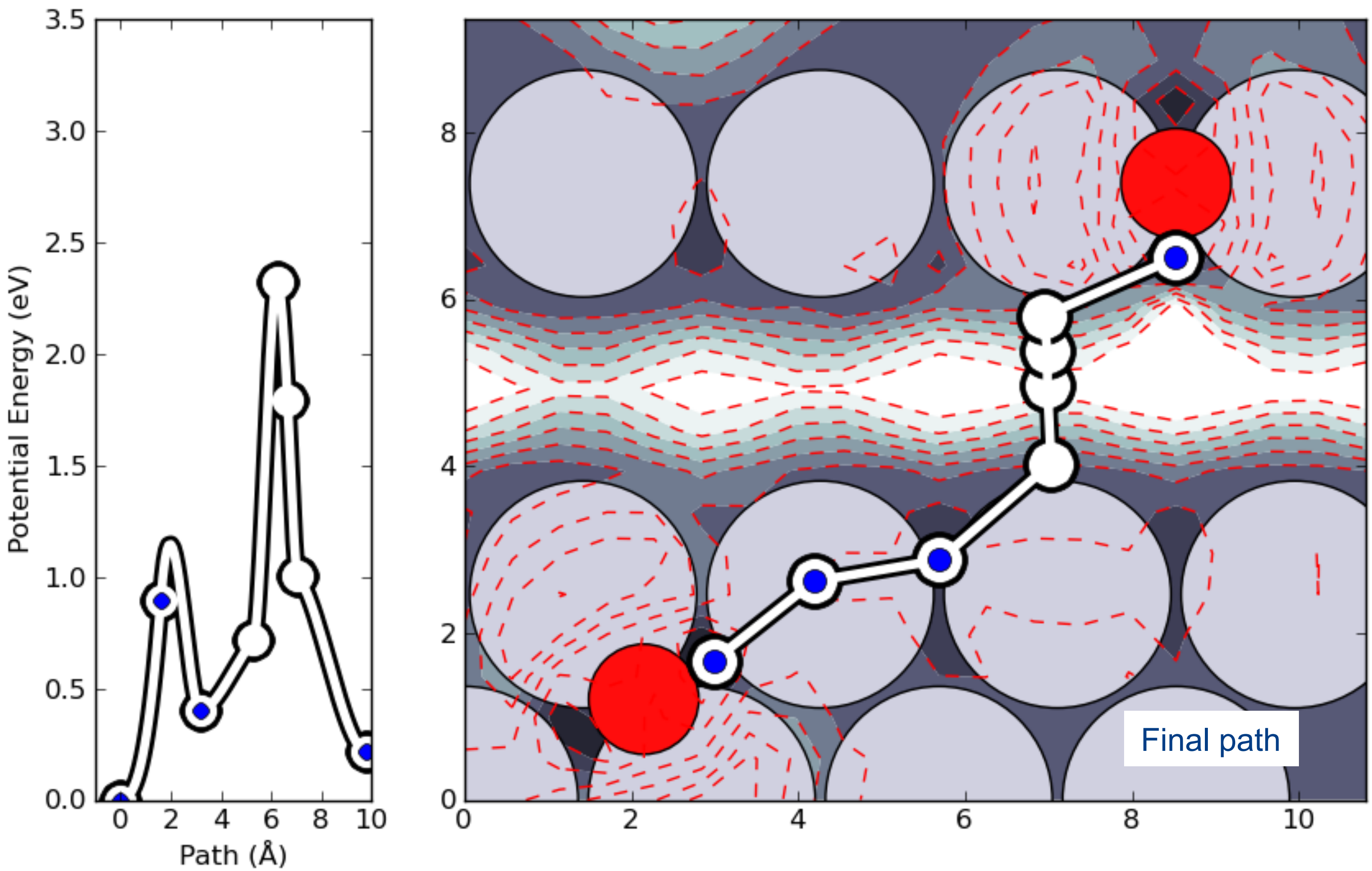


# Success 2: Climbing NEB

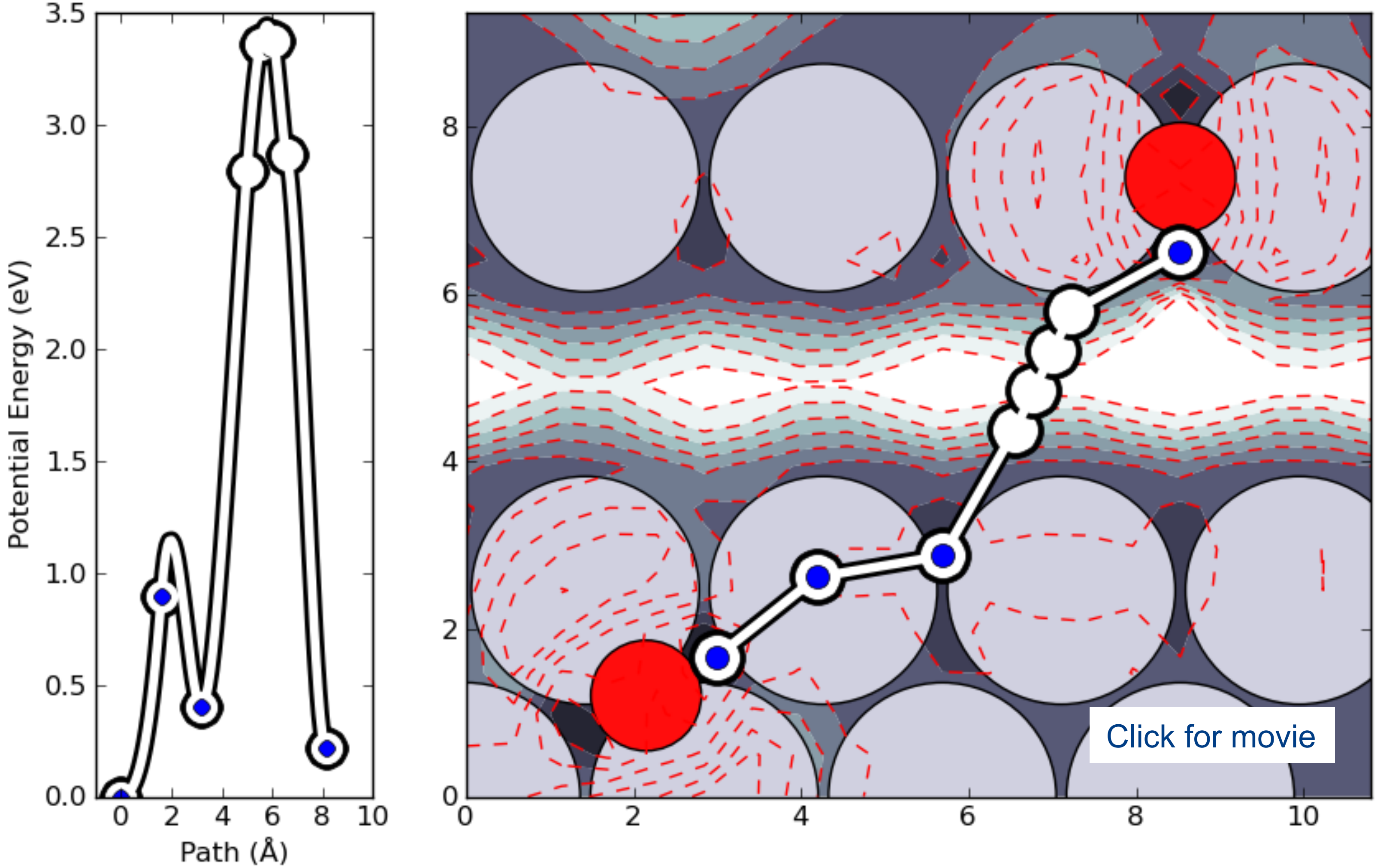


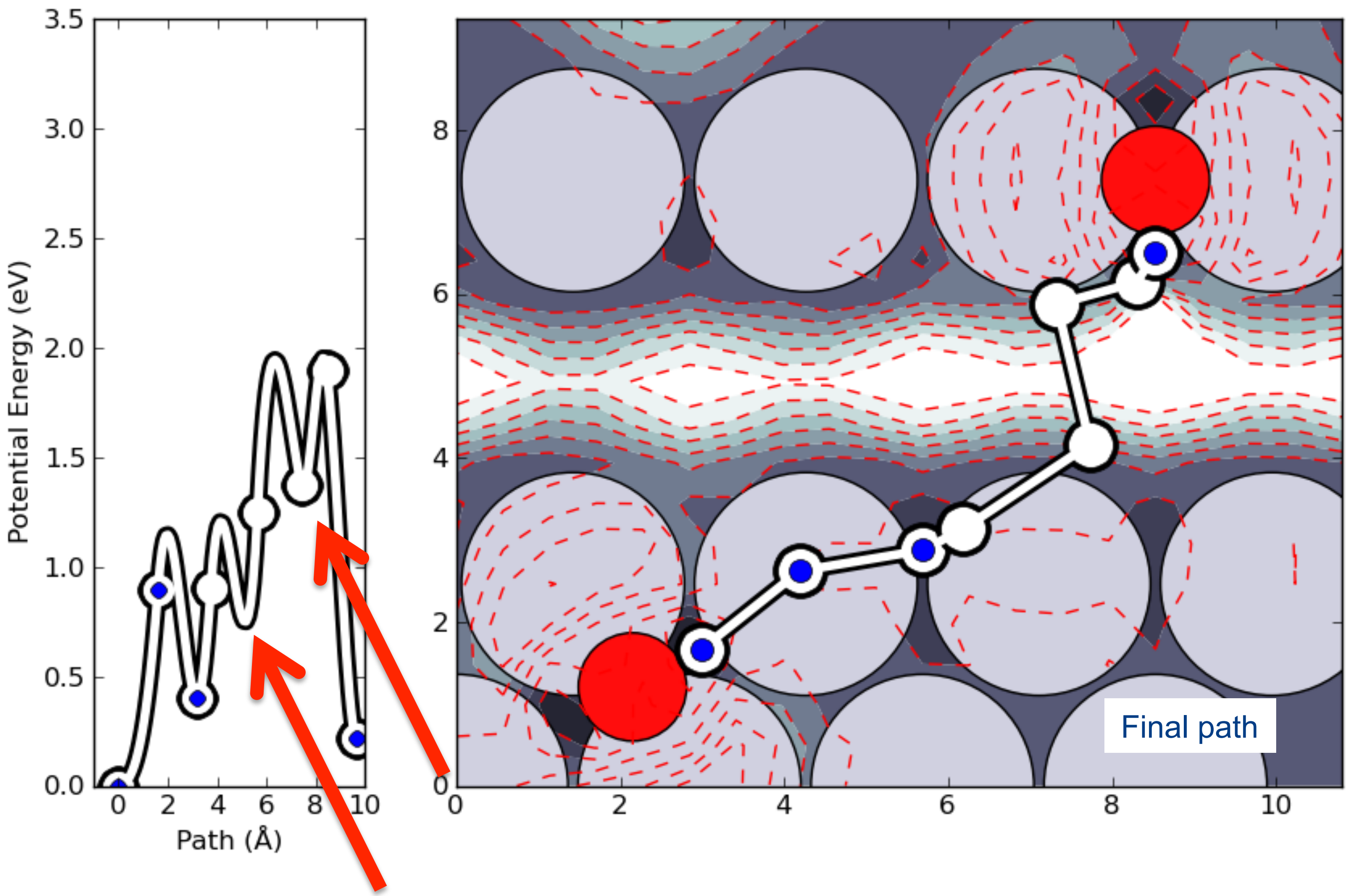
# Success 2: Climbing NEB



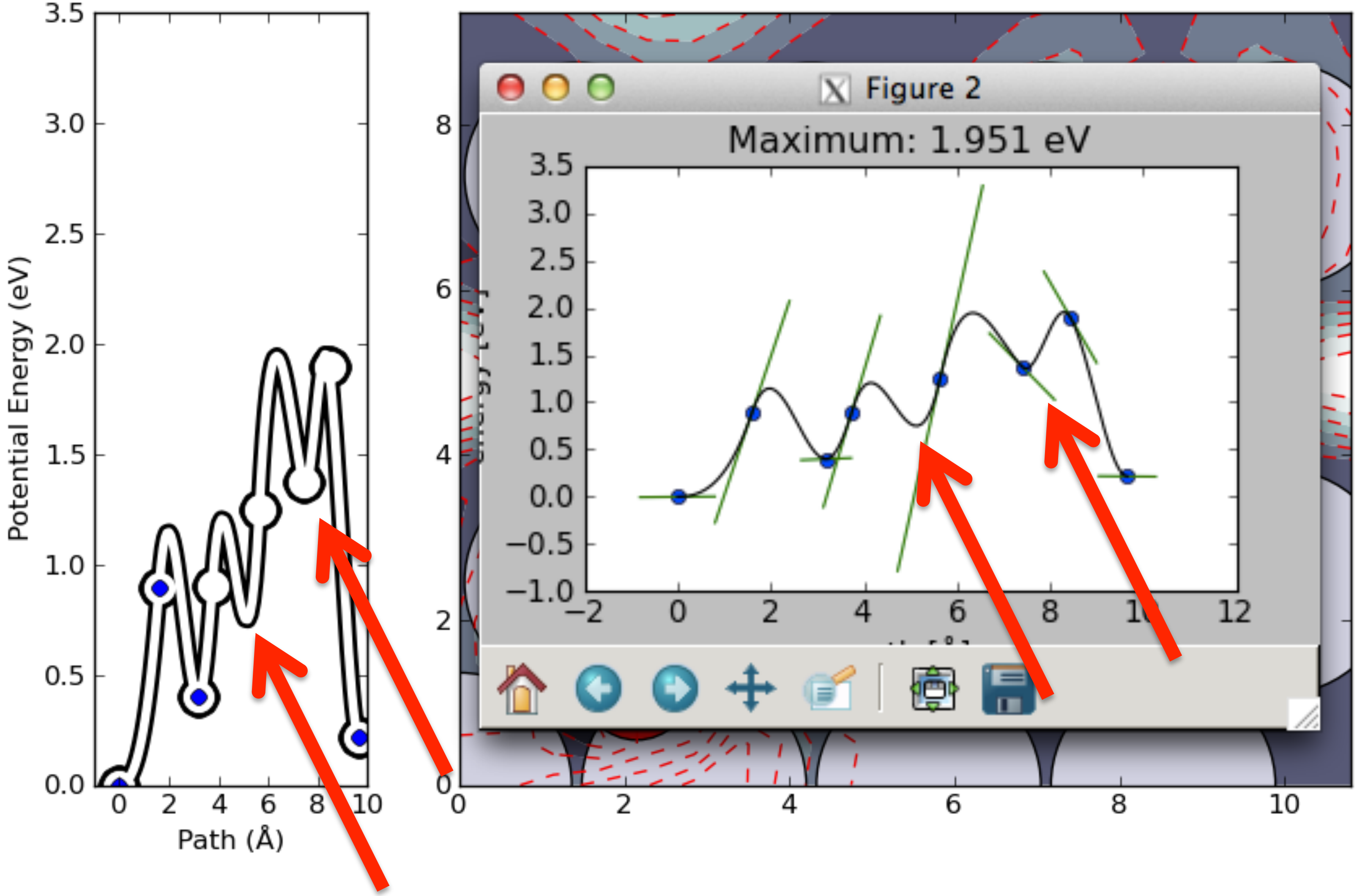
# Failure 1: Continued NEB



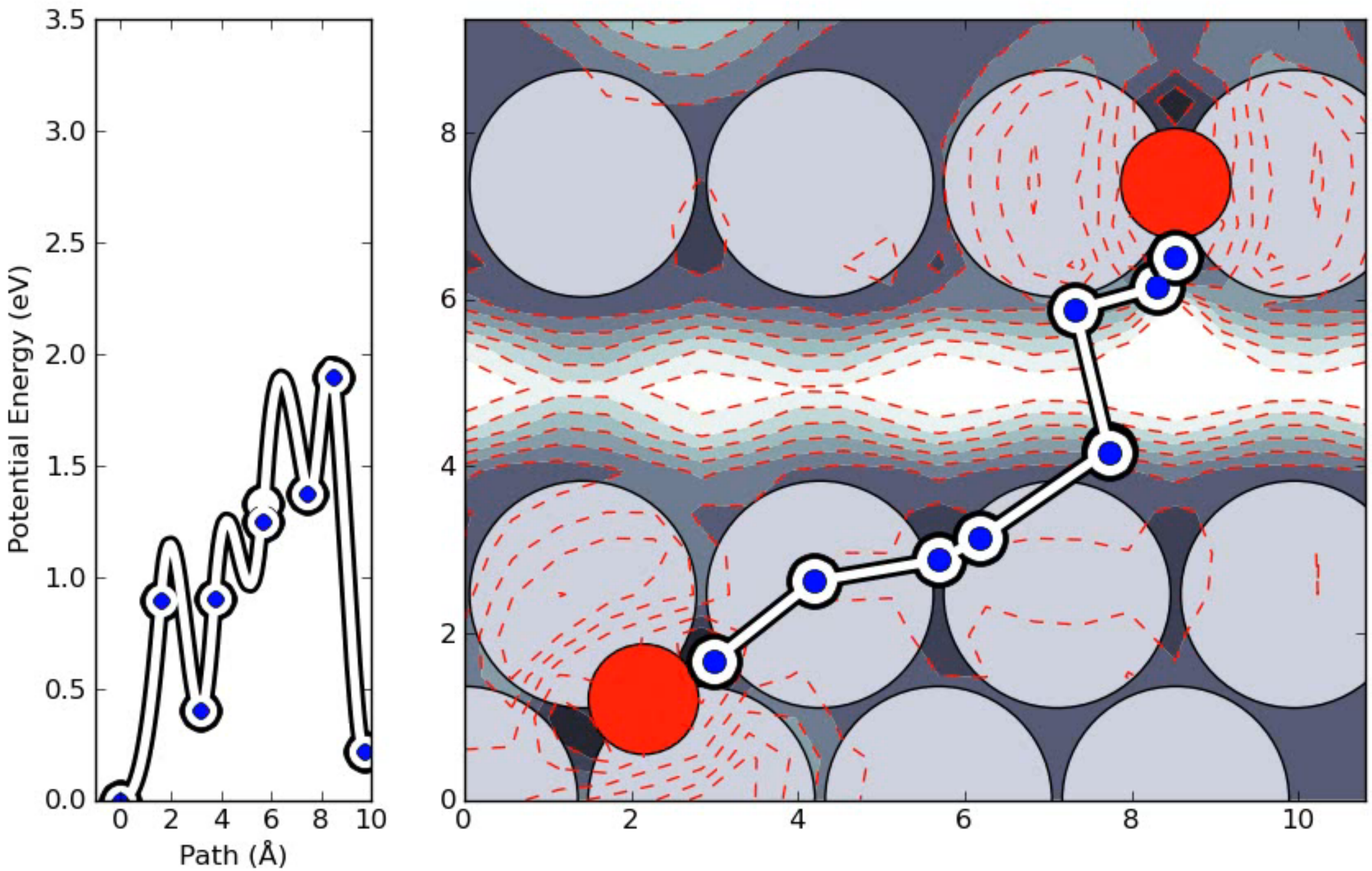
# Failure 1: Two new local minima



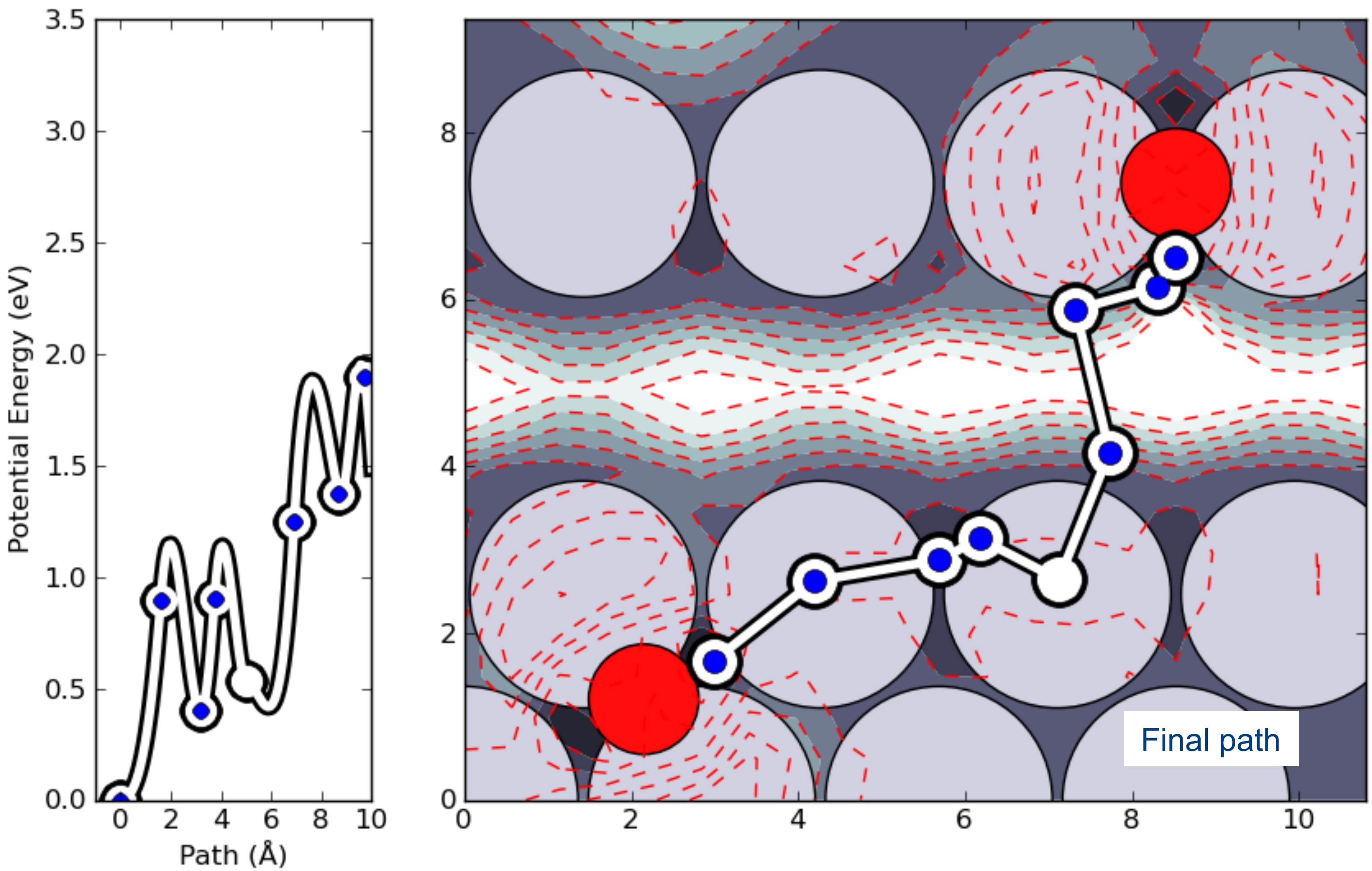
# Failure 1: Two new local minima



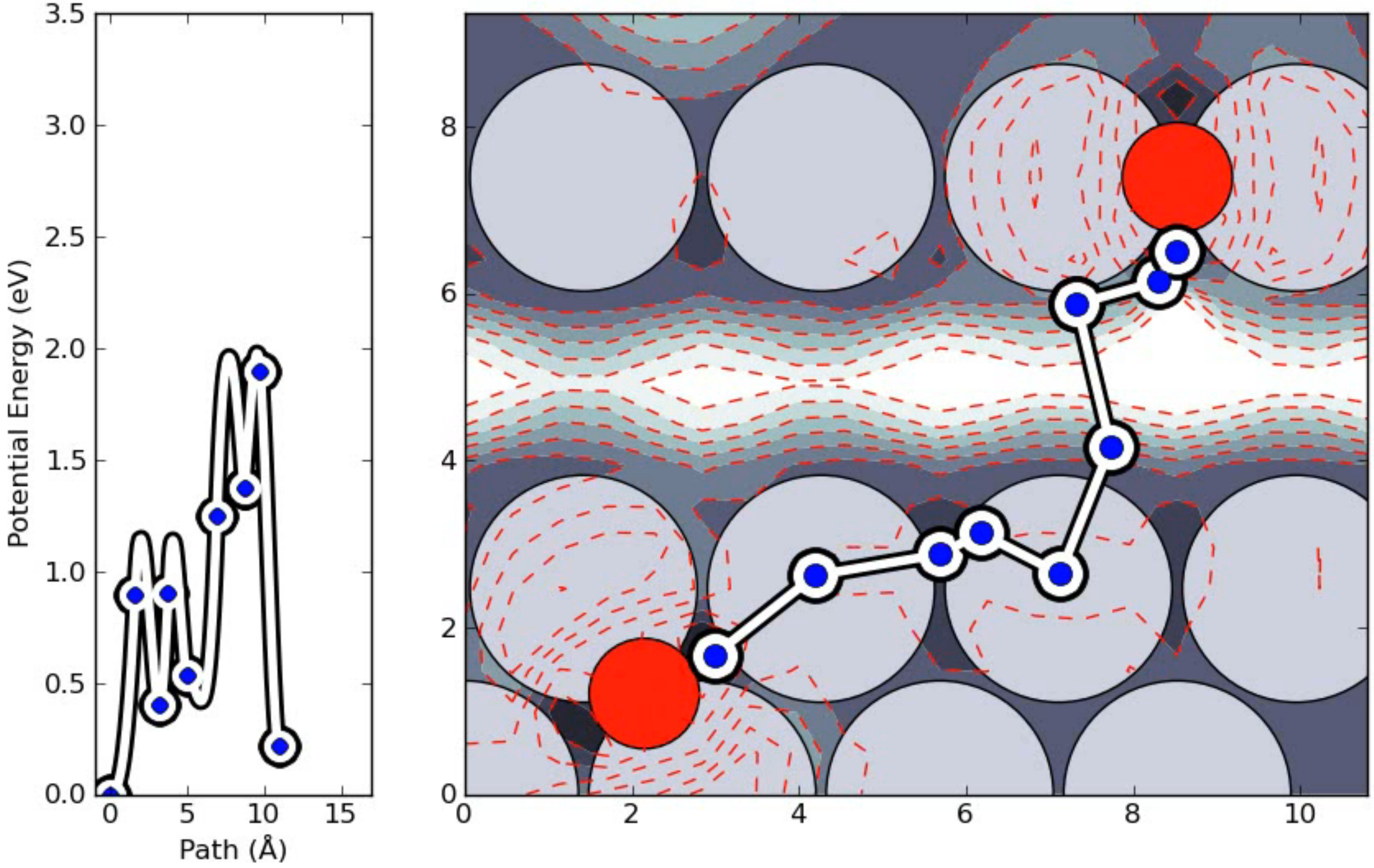
# Failure 1: Finding the first local minimum



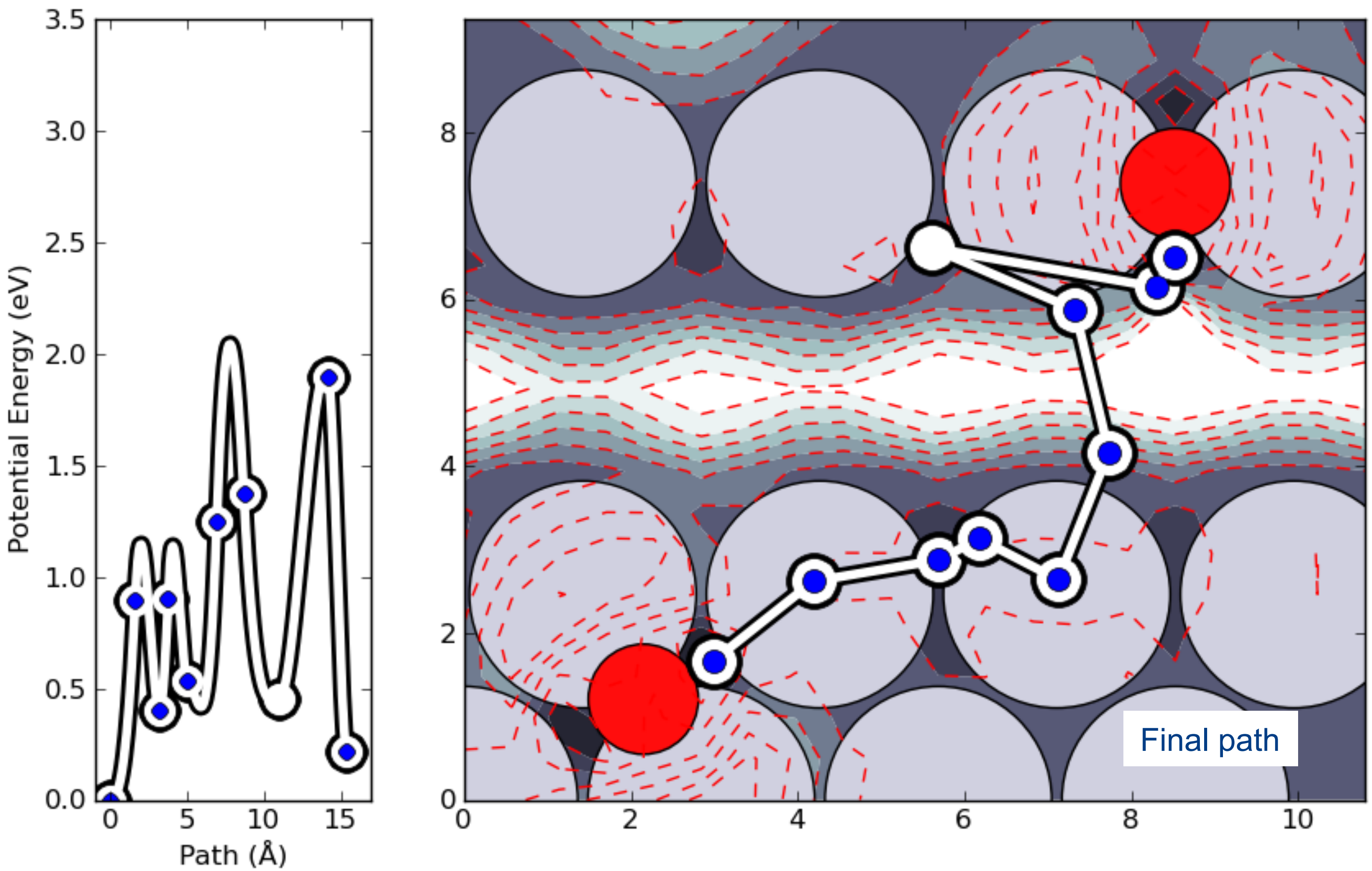
# Failure 1: Finding the first local minimum



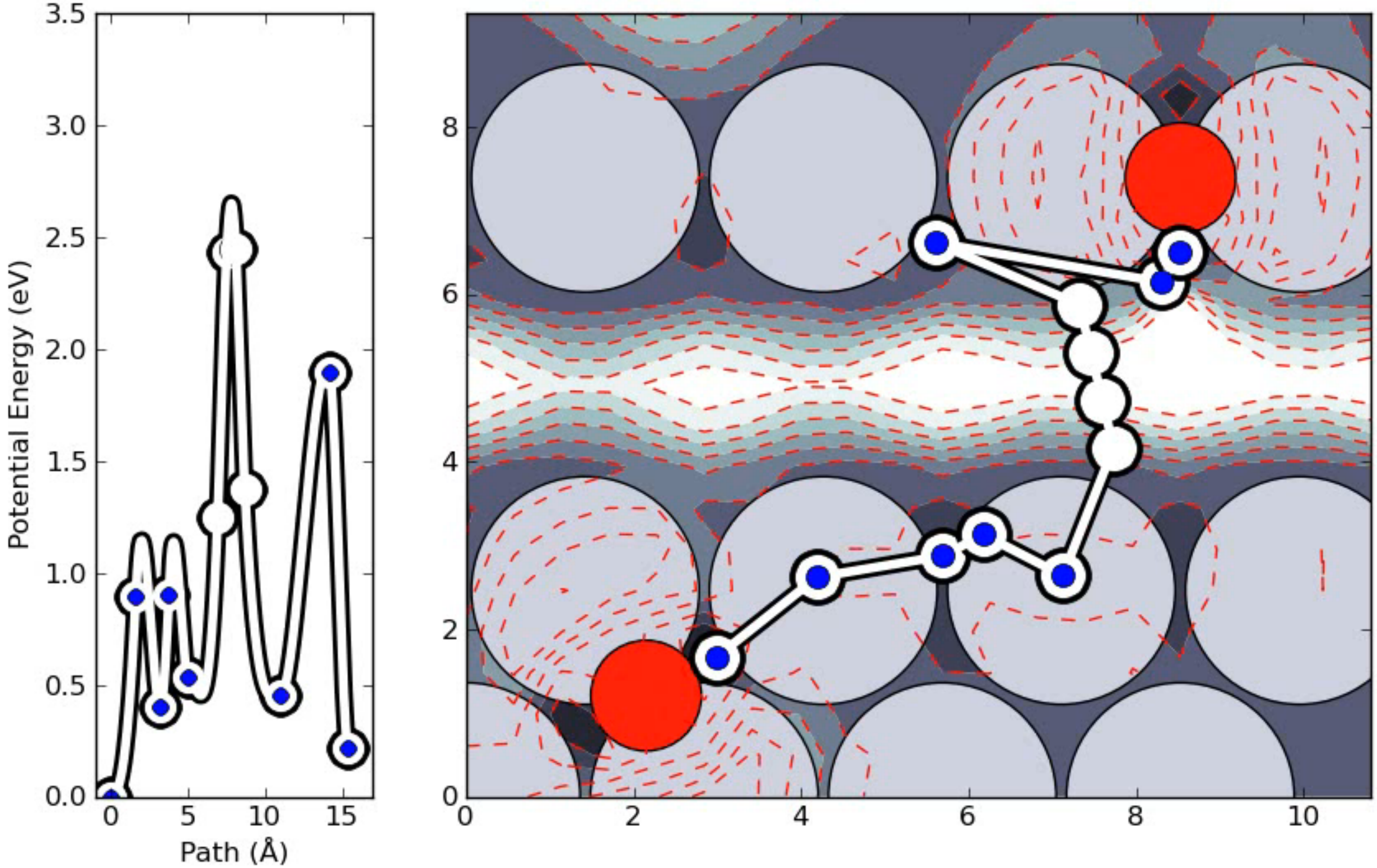
# Failure 1: Finding the 2nd local minimum



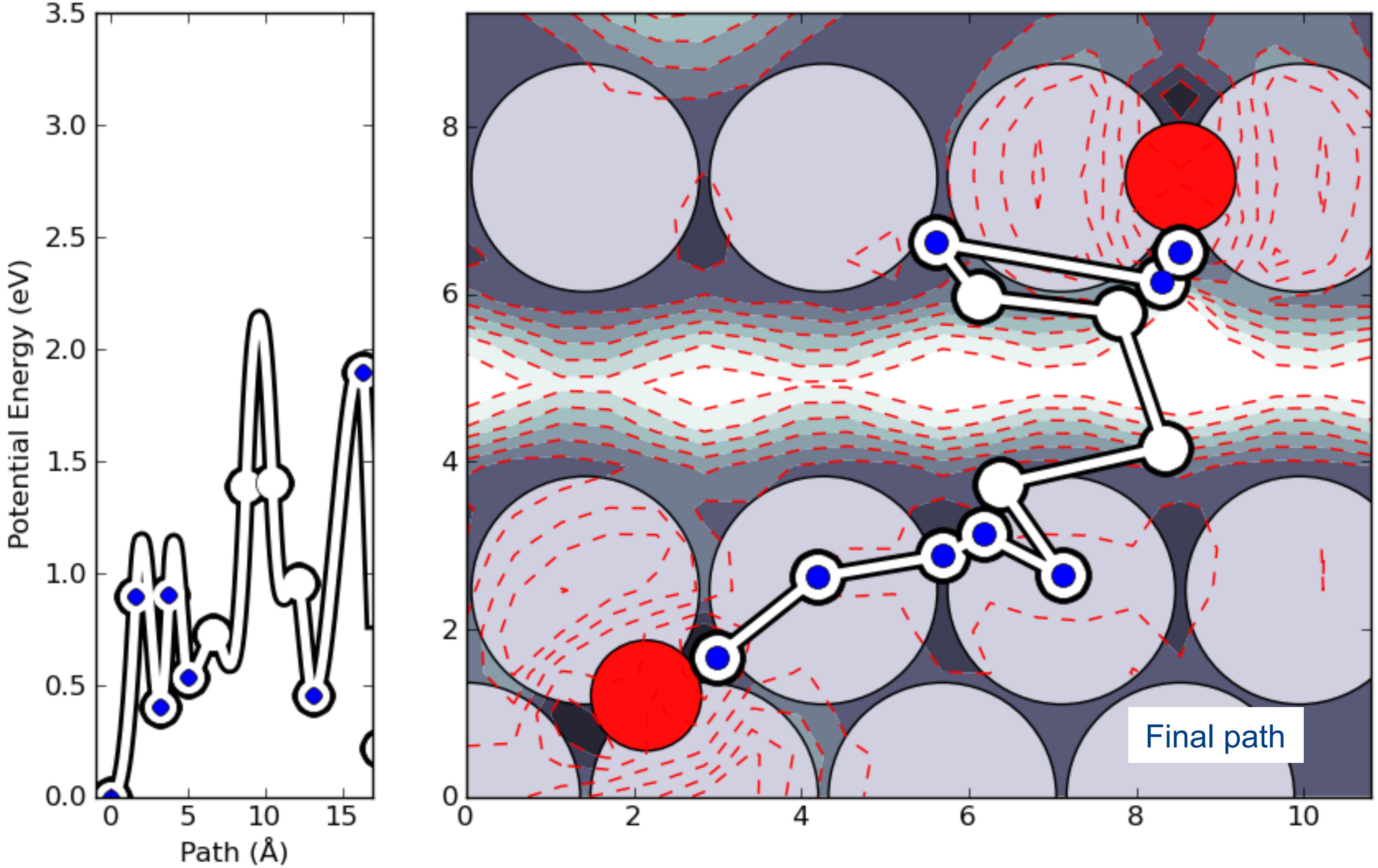
# Failure 1: Finding the 2nd local minimum



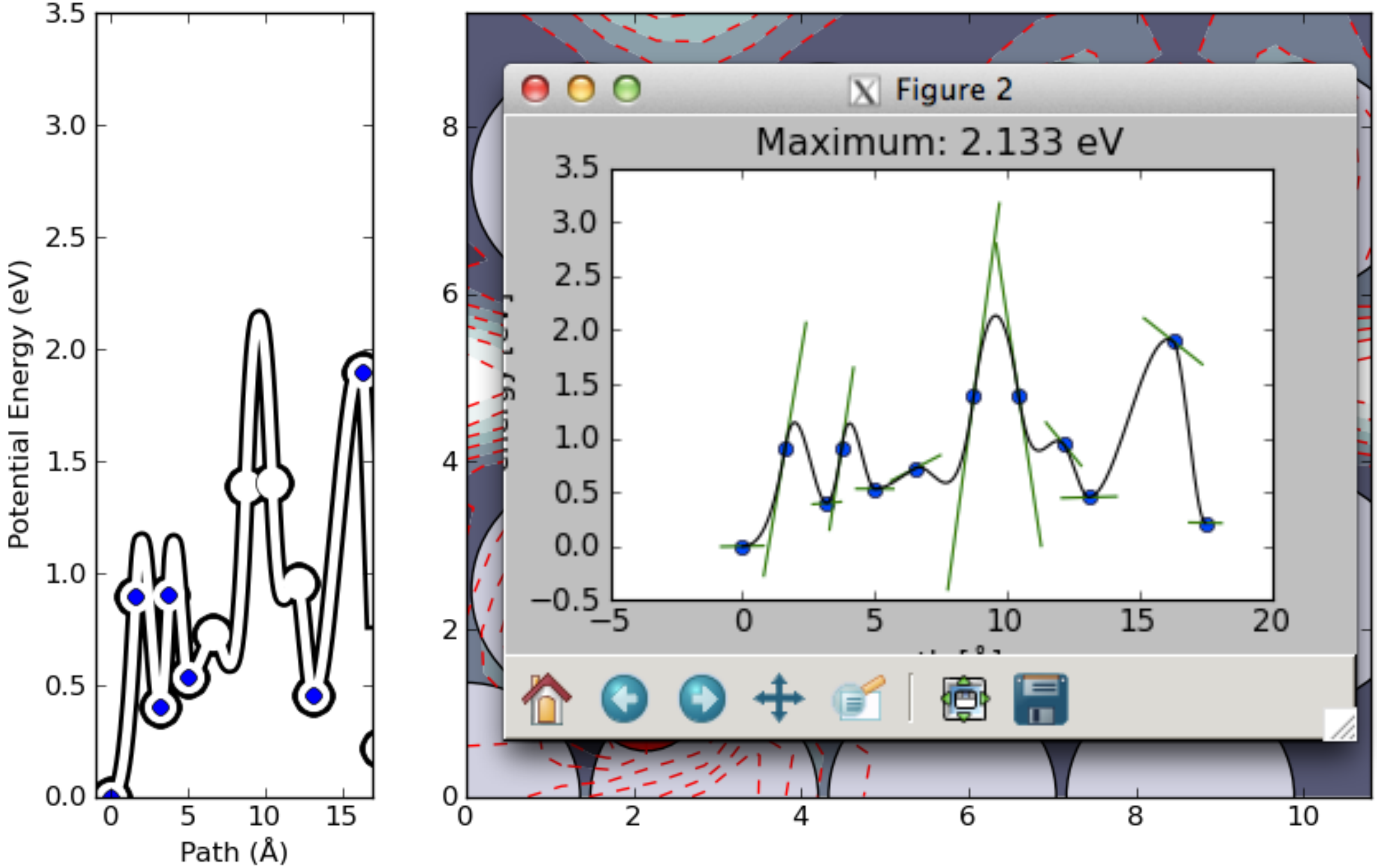
# Failure 1: NEB between new minima



# Failure 1: NEB between new minima



# Failure 1: NEB between new minima

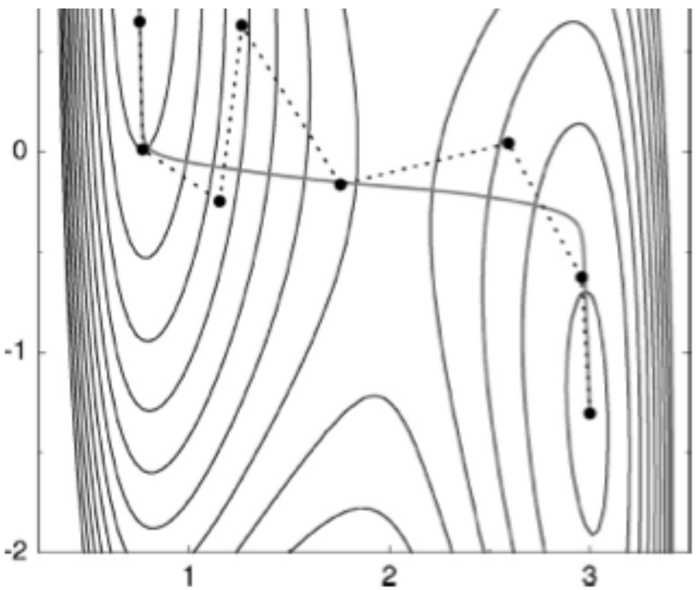


JOURNAL OF CHEMICAL PHYSICS VOLUME 113, NUMBER 22 8 DECEMBER 2000

# Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points

Graeme Henkelman[a] and Hannes Jónsson[b]
*Department of Chemistry, Box 351700, University of Washin*

$$\boldsymbol{\tau}_i = \frac{\mathbf{R}_i - \mathbf{R}_{i-1}}{|\mathbf{R}_i - \mathbf{R}_{i-1}|} + \frac{\mathbf{R}_{i+1} - \mathbf{R}_i}{|\mathbf{R}_{i+1} - \mathbf{R}_i|},$$

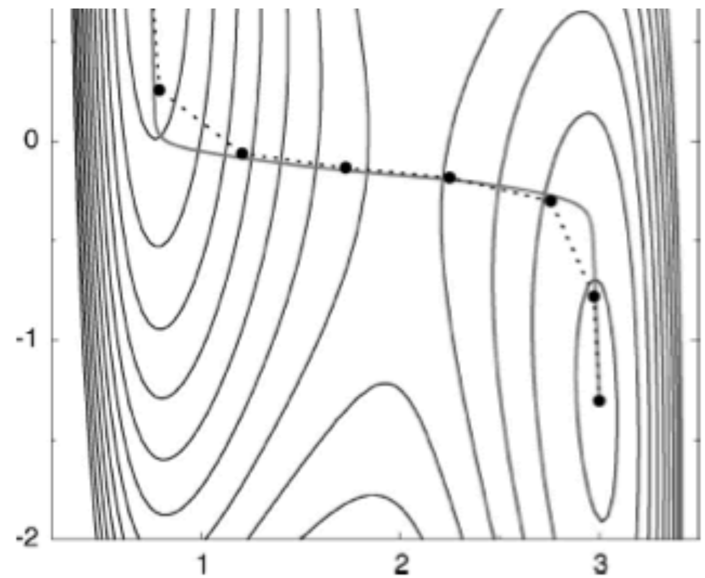



$$\mathbf{F}_i^s|_{\parallel} = k[(\mathbf{R}_{i+1} - \mathbf{R}_i) - (\mathbf{R}_i - \mathbf{R}_{i-1})] \cdot \hat{\boldsymbol{\tau}}_i \hat{\boldsymbol{\tau}}_i$$

$$\boldsymbol{\tau}_i = \begin{cases} \boldsymbol{\tau}_i^+ & \text{if} \quad V_{i+1} > V_i > V_{i-1} \\ \boldsymbol{\tau}_i^- & \text{if} \quad V_{i+1} < V_i < V_{i-1} \end{cases},$$

where

$$\boldsymbol{\tau}_i^+ = \mathbf{R}_{i+1} - \mathbf{R}_i, \quad \text{and} \quad \boldsymbol{\tau}_i^- = \mathbf{R}_i - \mathbf{R}_{i-1},$$




$$\mathbf{F}_i^s|_{\parallel} = k(|\mathbf{R}_{i+1} - \mathbf{R}_i| - |\mathbf{R}_i - \mathbf{R}_{i-1}|) \hat{\boldsymbol{\tau}}_i$$

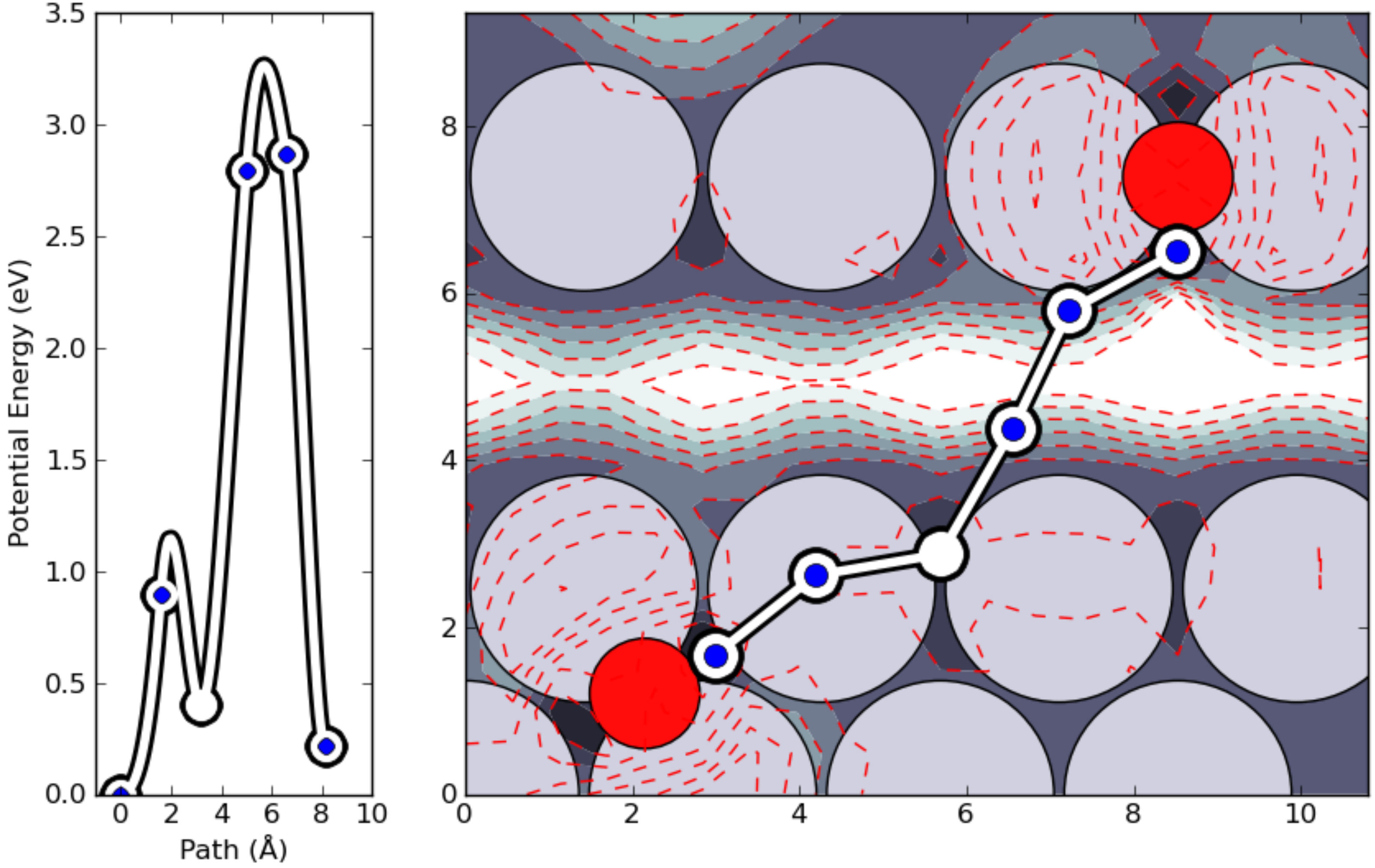
# ASE version / neb.py code

```
[hammer@fe1 gapneb]$ ls -otr ~/DFT/ase
lrwxrwxrwx 1 hammer 9 15 jan 11:52 /home/hammer/DFT/ase -> ase-3.6.0
[hammer@fe1 gapneb]$
```

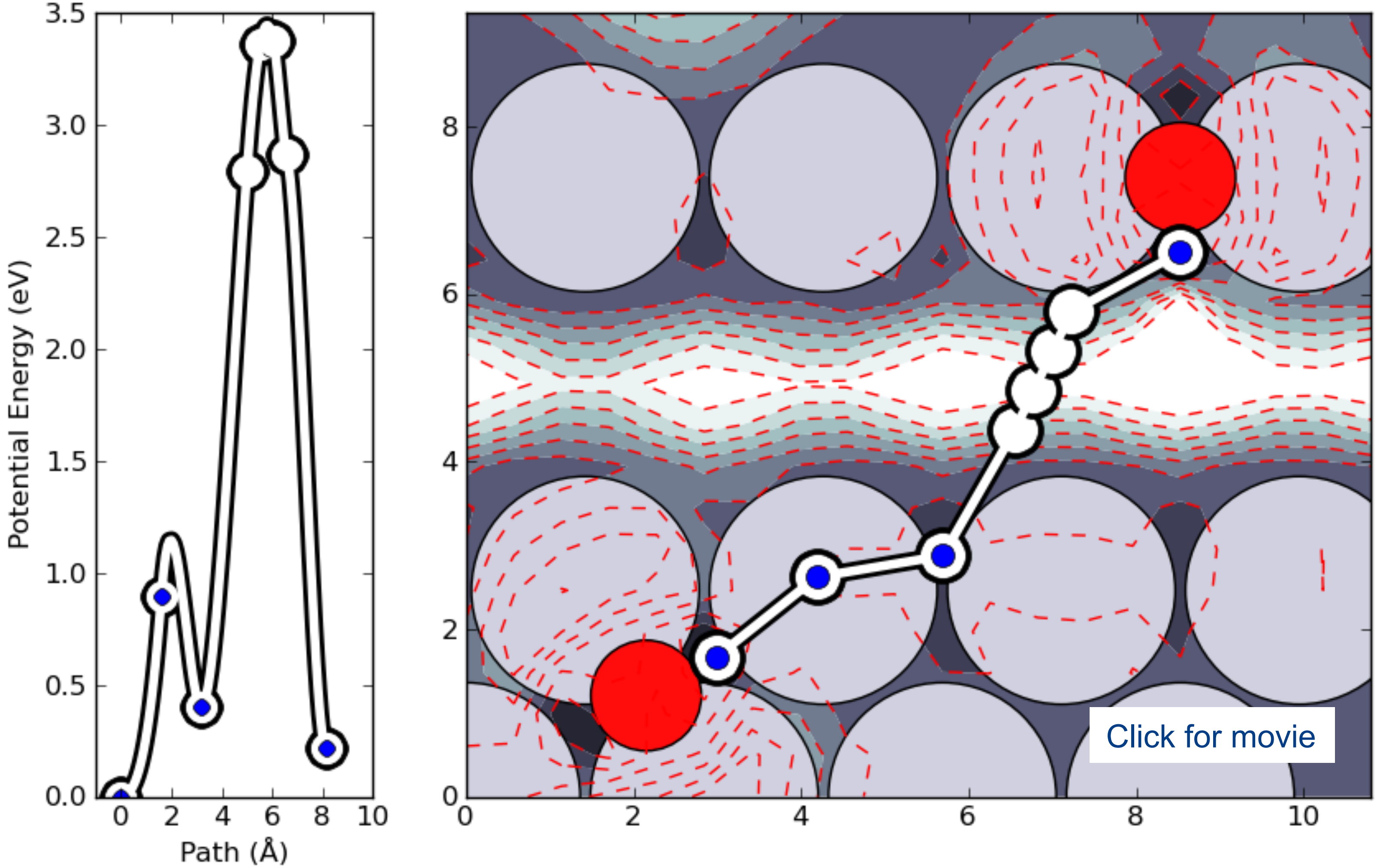
```
imax = 1 + np.argsort(energies)[-1]
self.emax = energies[imax - 1]

tangent1 = images[1].get_positions() - images[0].get_positions()
for i in range(1, self.nimages - 1):
    tangent2 = (images[i + 1].get_positions() -
                images[i].get_positions())
    if i < imax:
        tangent = tangent2
    elif i > imax:
        tangent = tangent1
    else:
        tangent = tangent1 + tangent2

    tt = np.vdot(tangent, tangent)
    f = forces[i - 1]
    ft = np.vdot(f, tangent)
    if i == imax and self.climb:
        f -= 2 * ft / tt * tangent
    else:
        f -= ft / tt * tangent
        f -= np.vdot(tangent1 * self.k[i - 1] -
                     tangent2 * self.k[i], tangent) / tt * tangent

    tangent1 = tangent2
```

$$\mathbf{F}_i^s\big|_{\parallel} = k[(\mathbf{R}_{i+1} - \mathbf{R}_i) - (\mathbf{R}_i - \mathbf{R}_{i-1})] \cdot \hat{\boldsymbol{\tau}}_i \hat{\boldsymbol{\tau}}_i$$

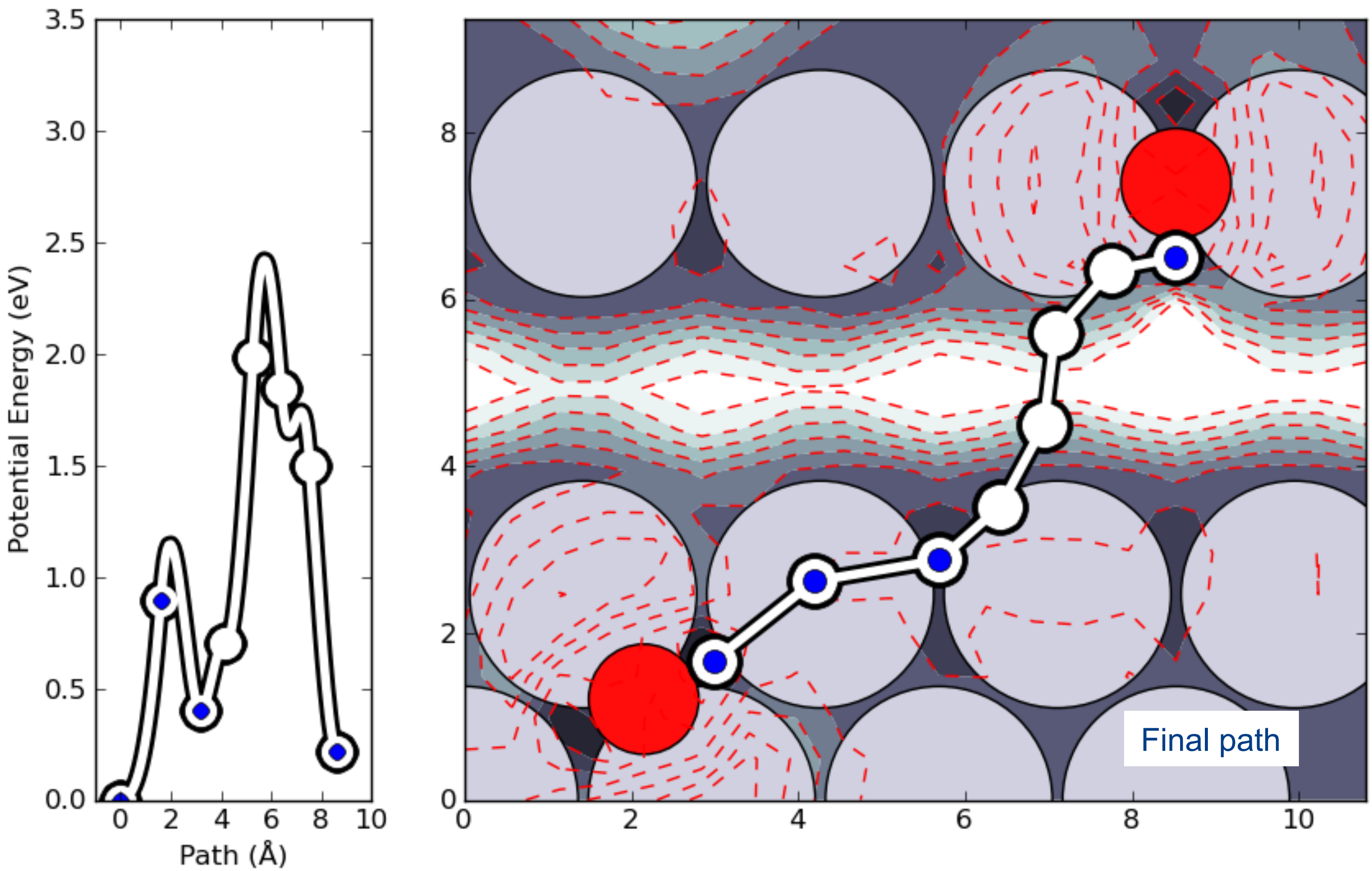
# Solution: spring-NEB



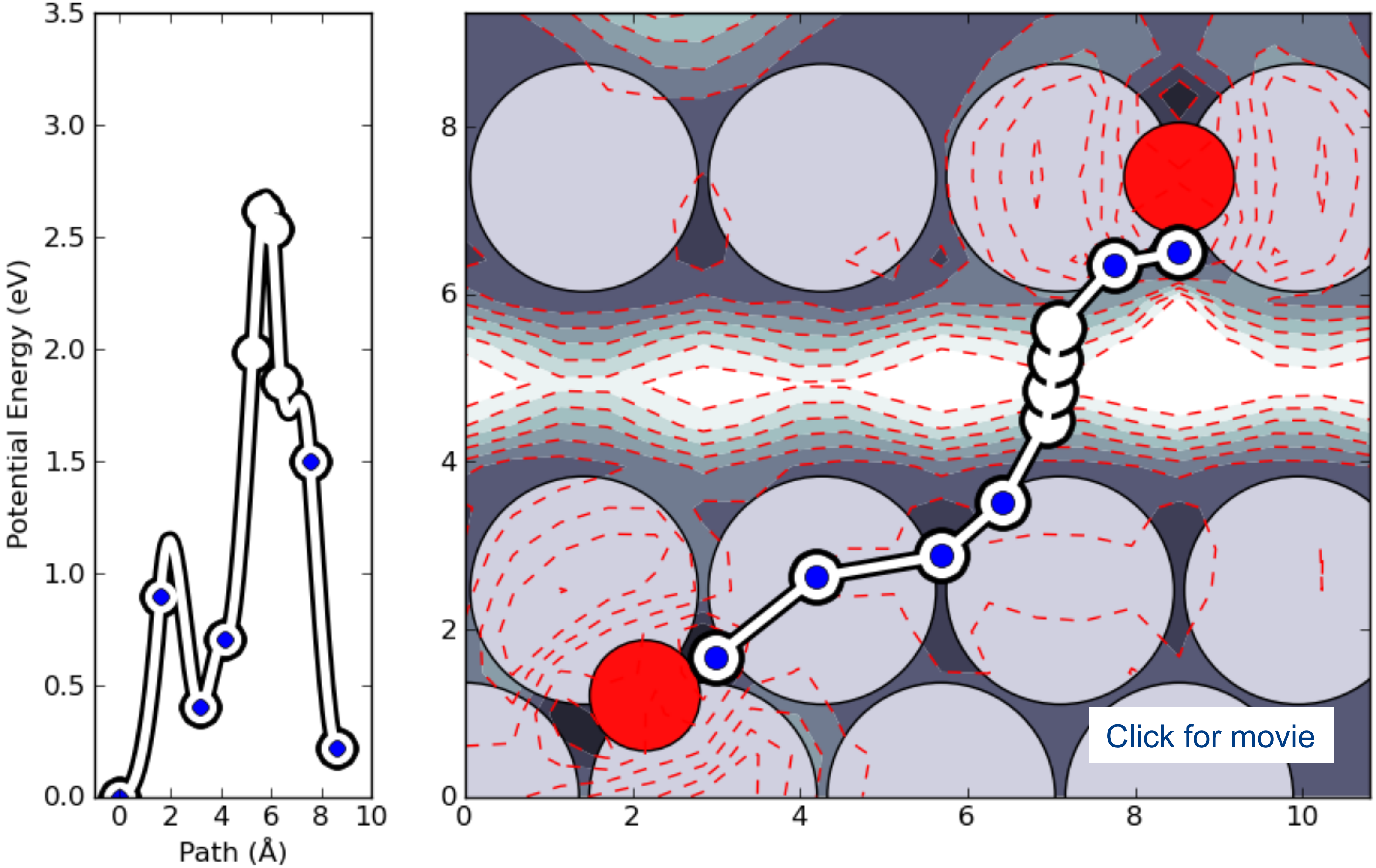
# Solution: spring-NEB



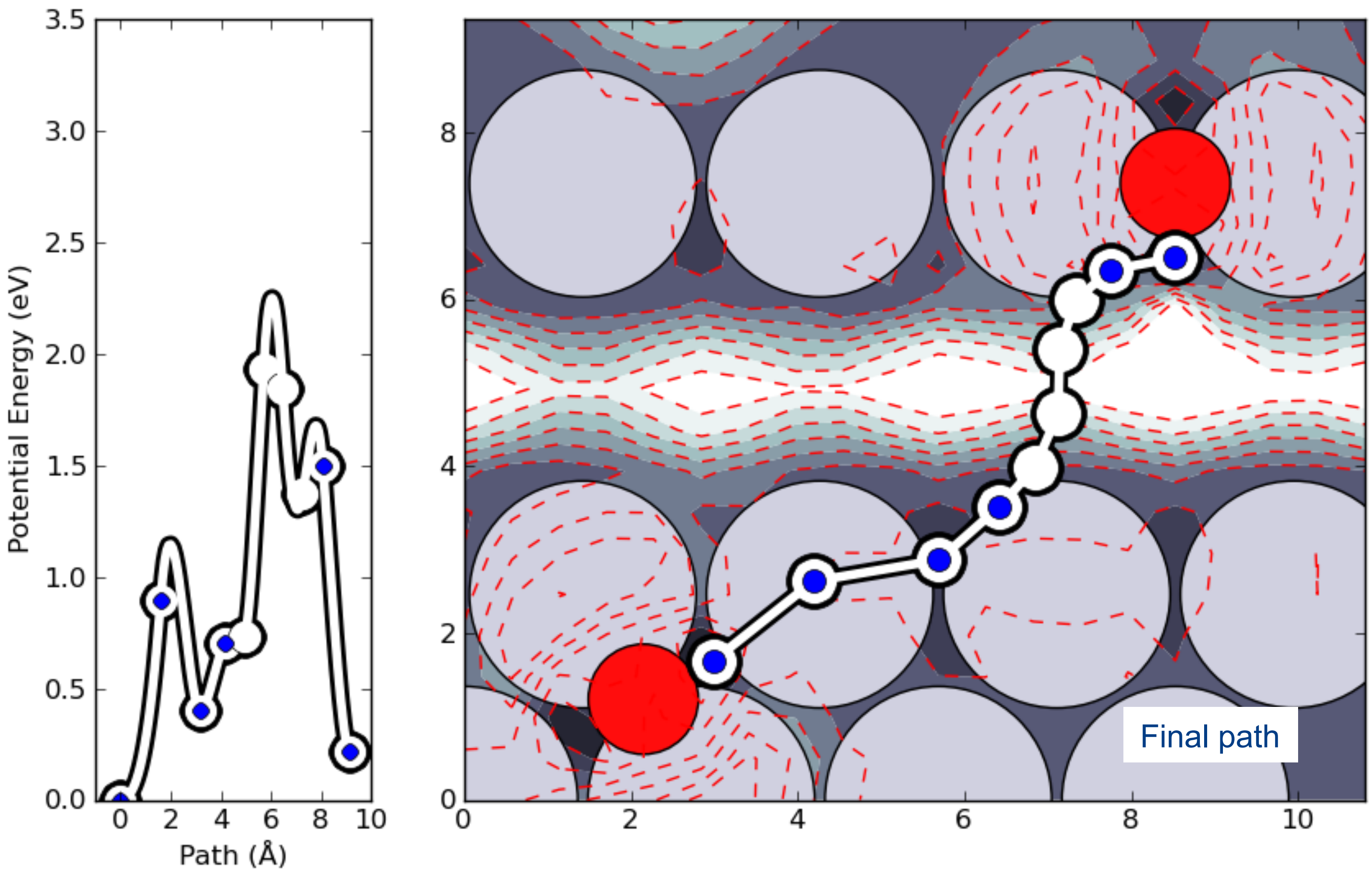
# Solution: spring-NEB



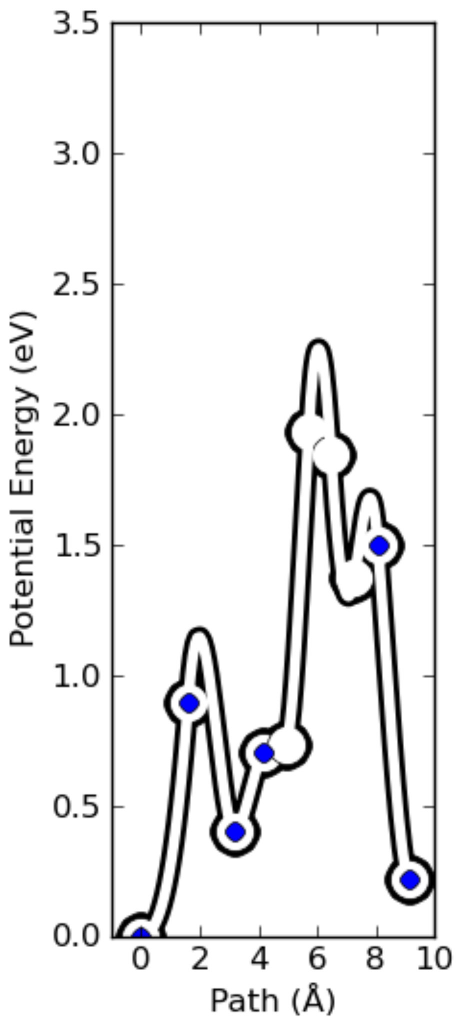
# Solution: spring-NEB

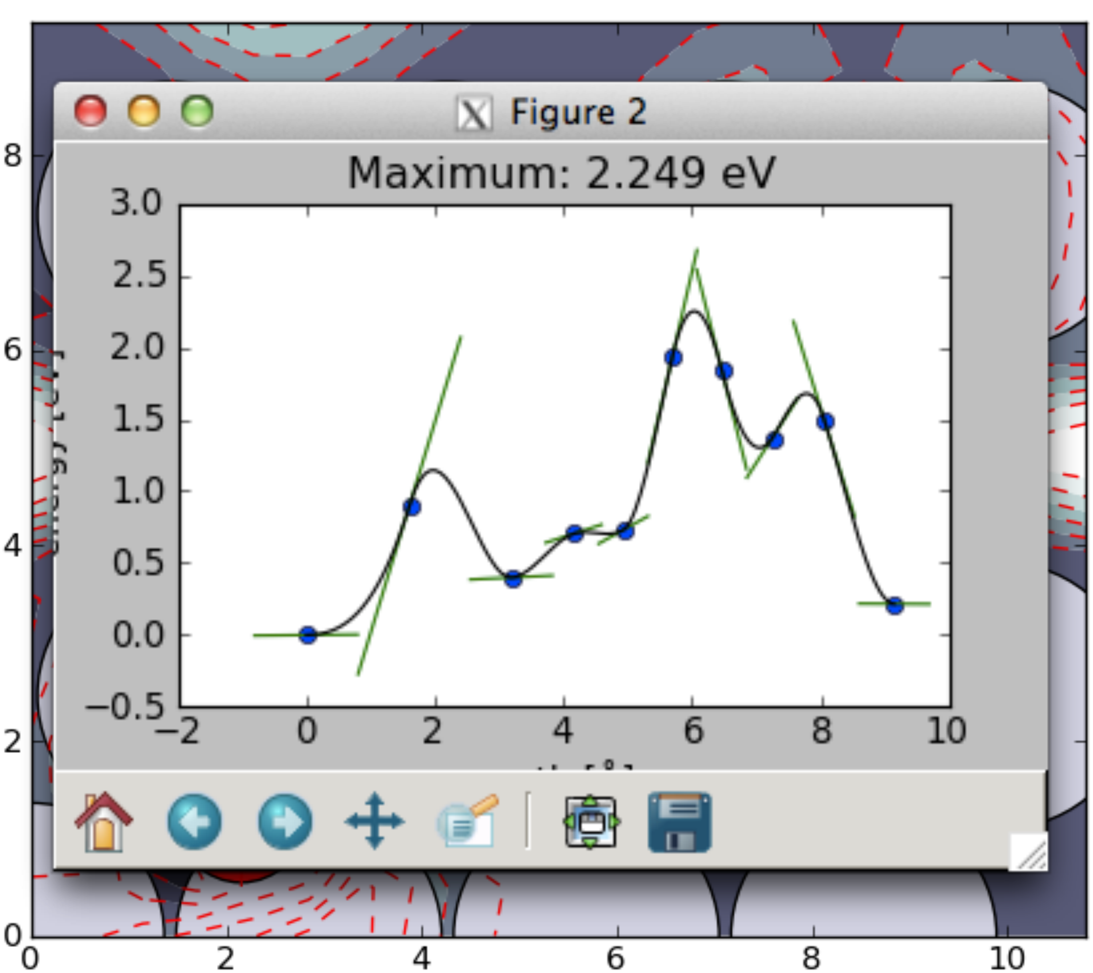


# Solution: spring-NEB

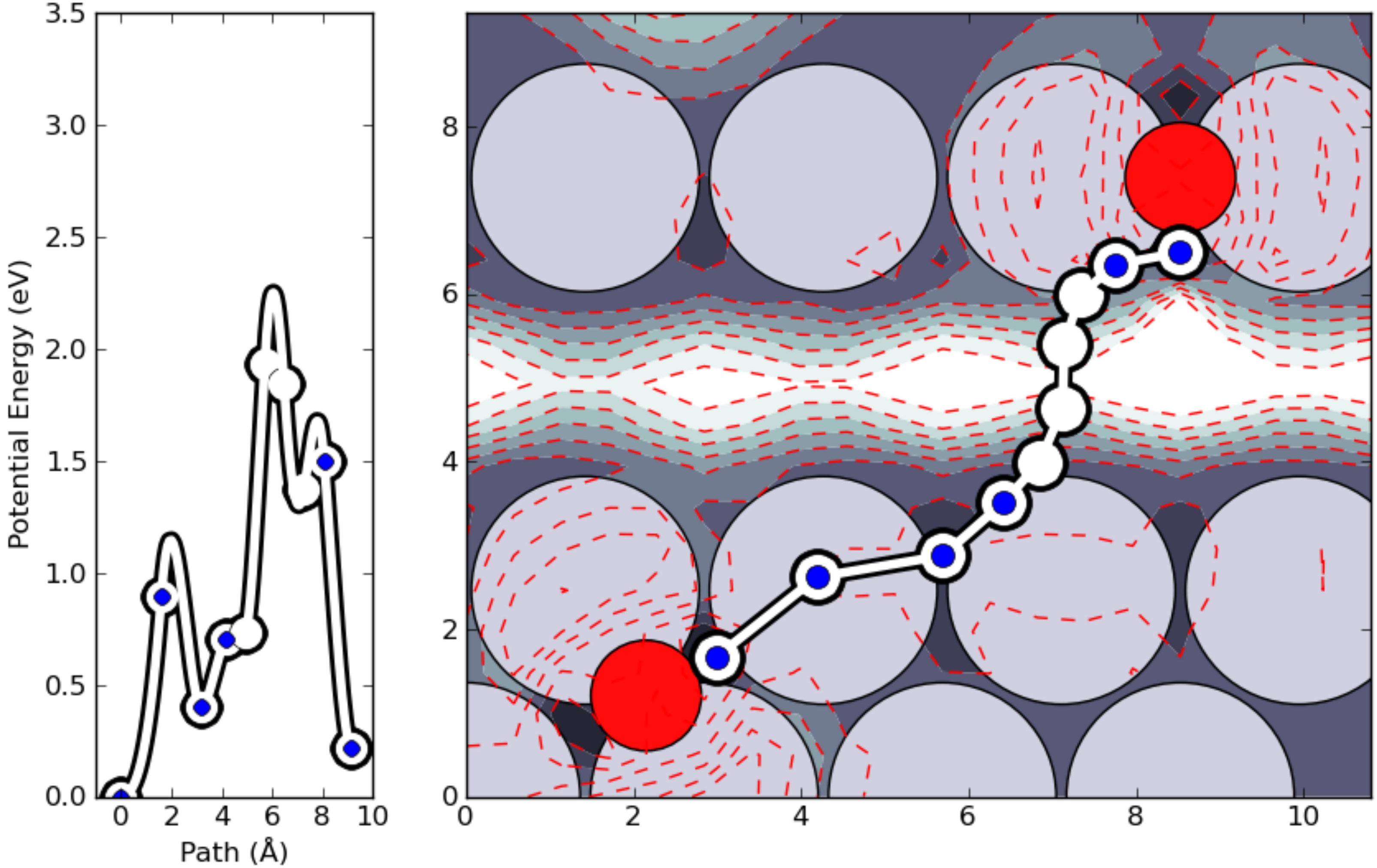


# Solution: spring-NEB

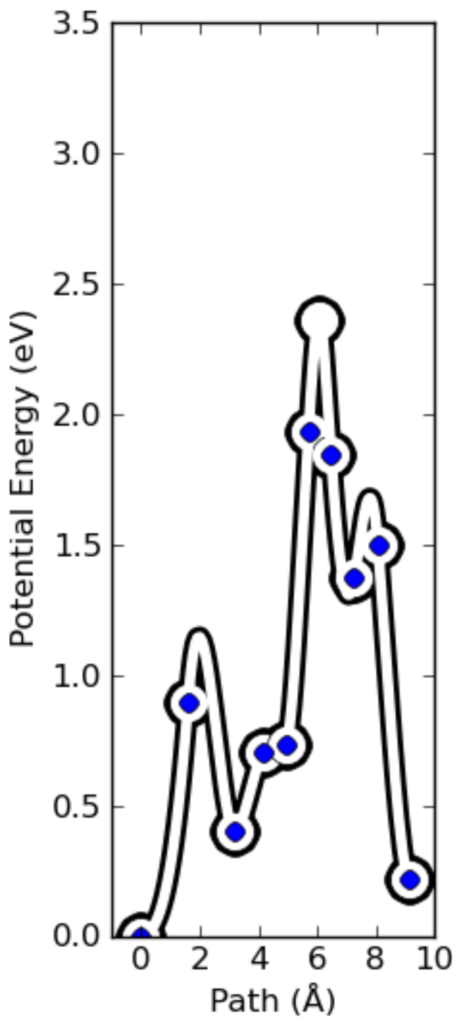


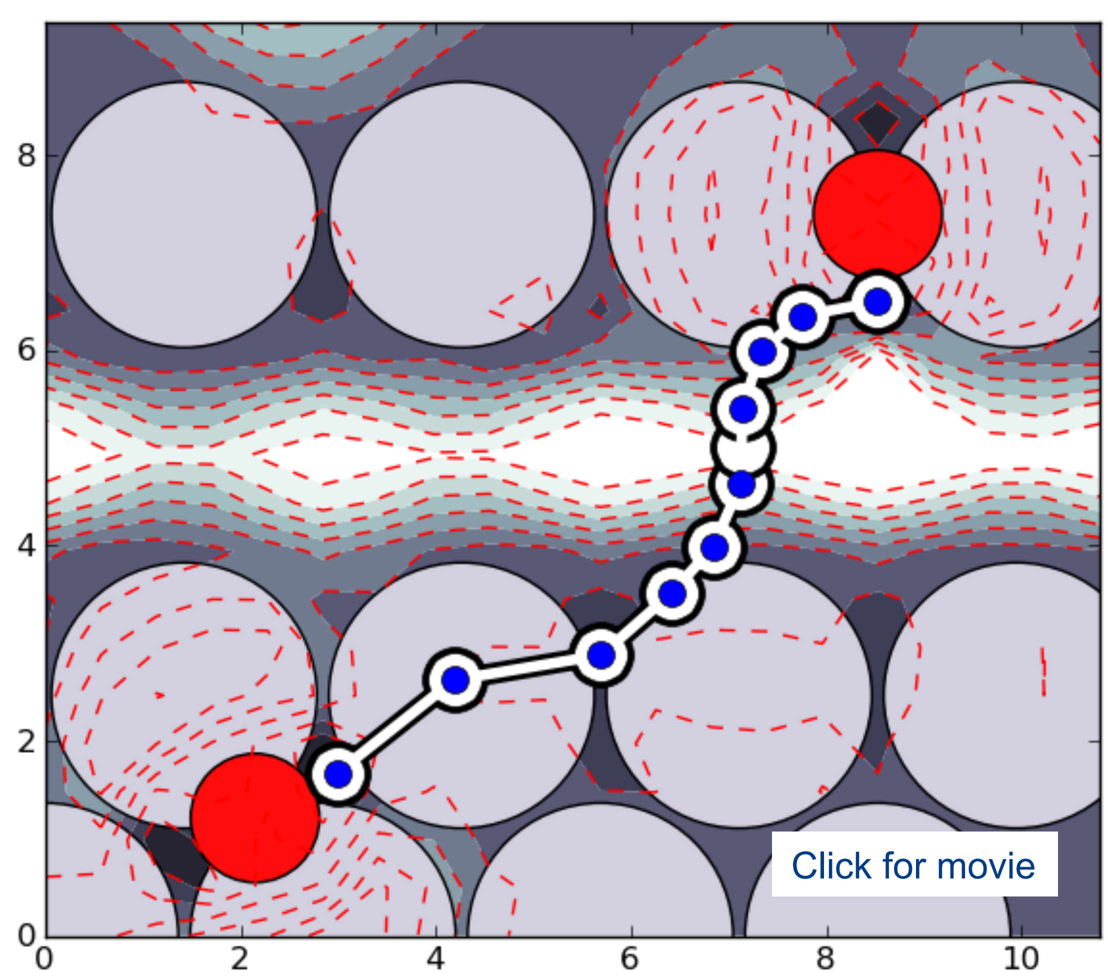



# Solution: spring-NEB

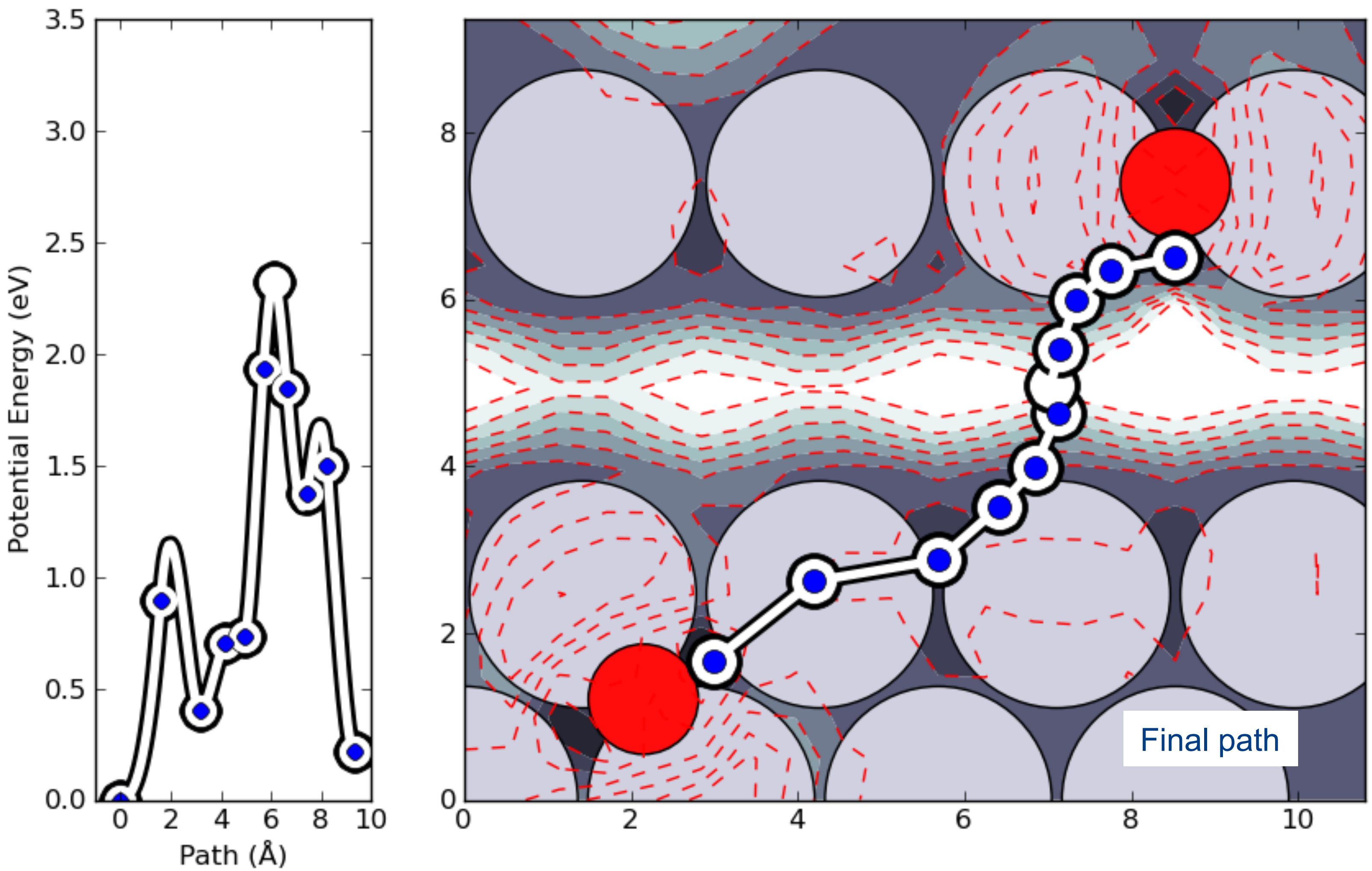


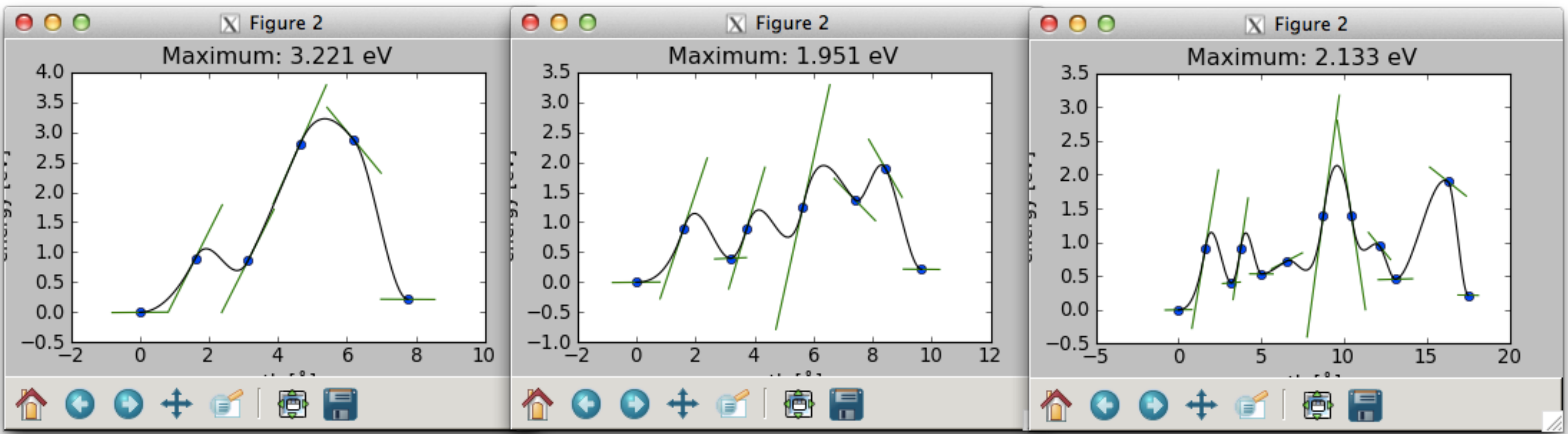
# Solution: spring-NEB + climbing-NEB



# Solution: spring-NEB + climbing-NEB

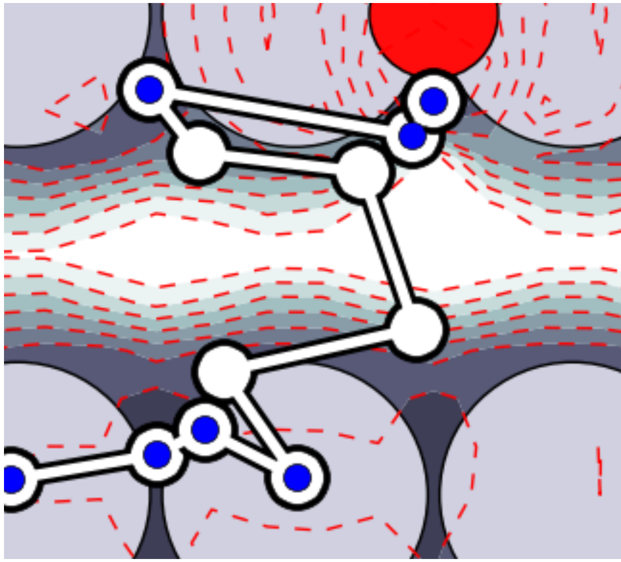





- Observation: finding saddle points with ASE is challenging.

- Problem: images may drift apart with:

$$\mathbf{F}_i^s\big|_{\parallel} = k\left(|\mathbf{R}_{i+1}-\mathbf{R}_i| - |\mathbf{R}_i-\mathbf{R}_{i-1}|\right)\hat{\boldsymbol{\tau}}_i$$



- Solution: reintroduce springs?