DIRECTED COLLISION OF $\vec{F}$ OR $\vec{CF}_2$ WITH CF_3(ad) GIVES UMBRELLA INVERSION OF CF_3(ad) FOLLOWED BY COLLINEAR EJECTION OF $\vec{F}$ OR $\vec{CF}_2$

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Overall Outline

Achieving Directed Collision with a 'Surface-Molecular-Beam'

- What is a 'Surface-Molecular-Beam' ?
- How to Direct a Collision: Selecting Impact Parameter

Experiment

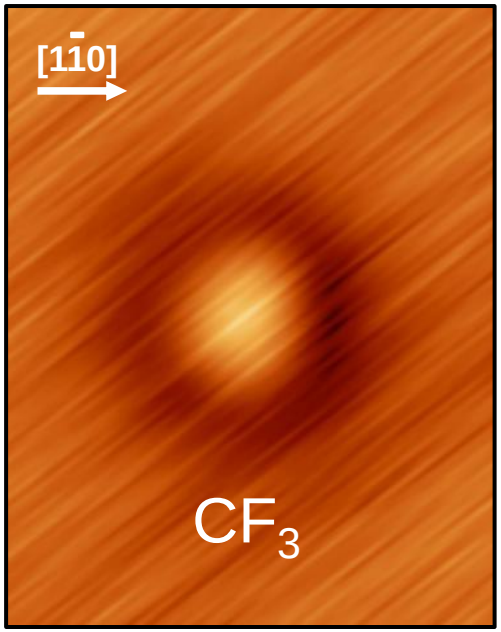
- Example 1: Directed Collision at **Three** Different Impact Parameters
- Example 2: Directed Collision at specifically **Zero** Impact Parameter ('Knock-On' Reaction) PRESENT WORK

Conclusions

What is a ‘Surface-Molecular-Beam’ ?

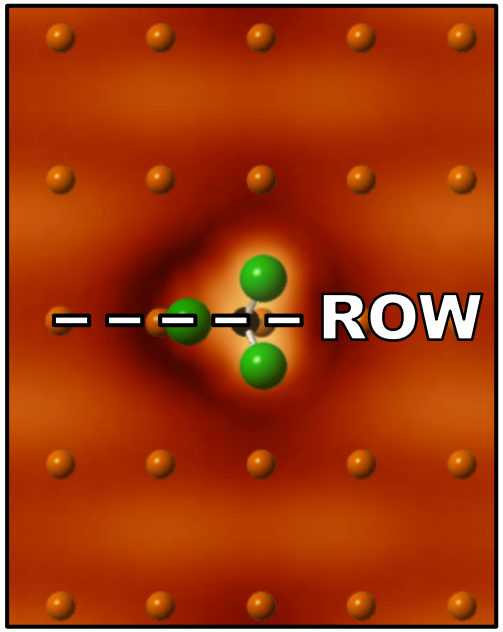
The Adsorbate: Trifluoromethyl (CF_3)

STM image

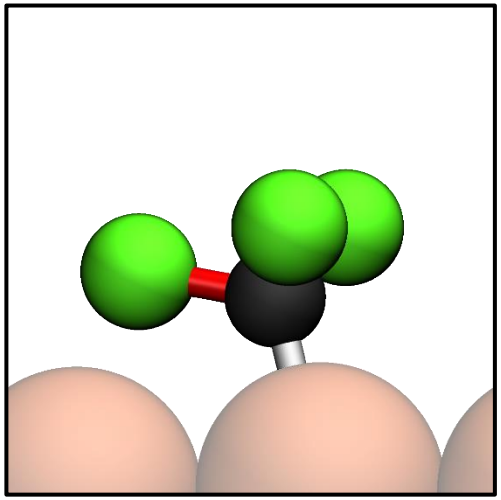


-50 mV, 50 pA, 4.6 K

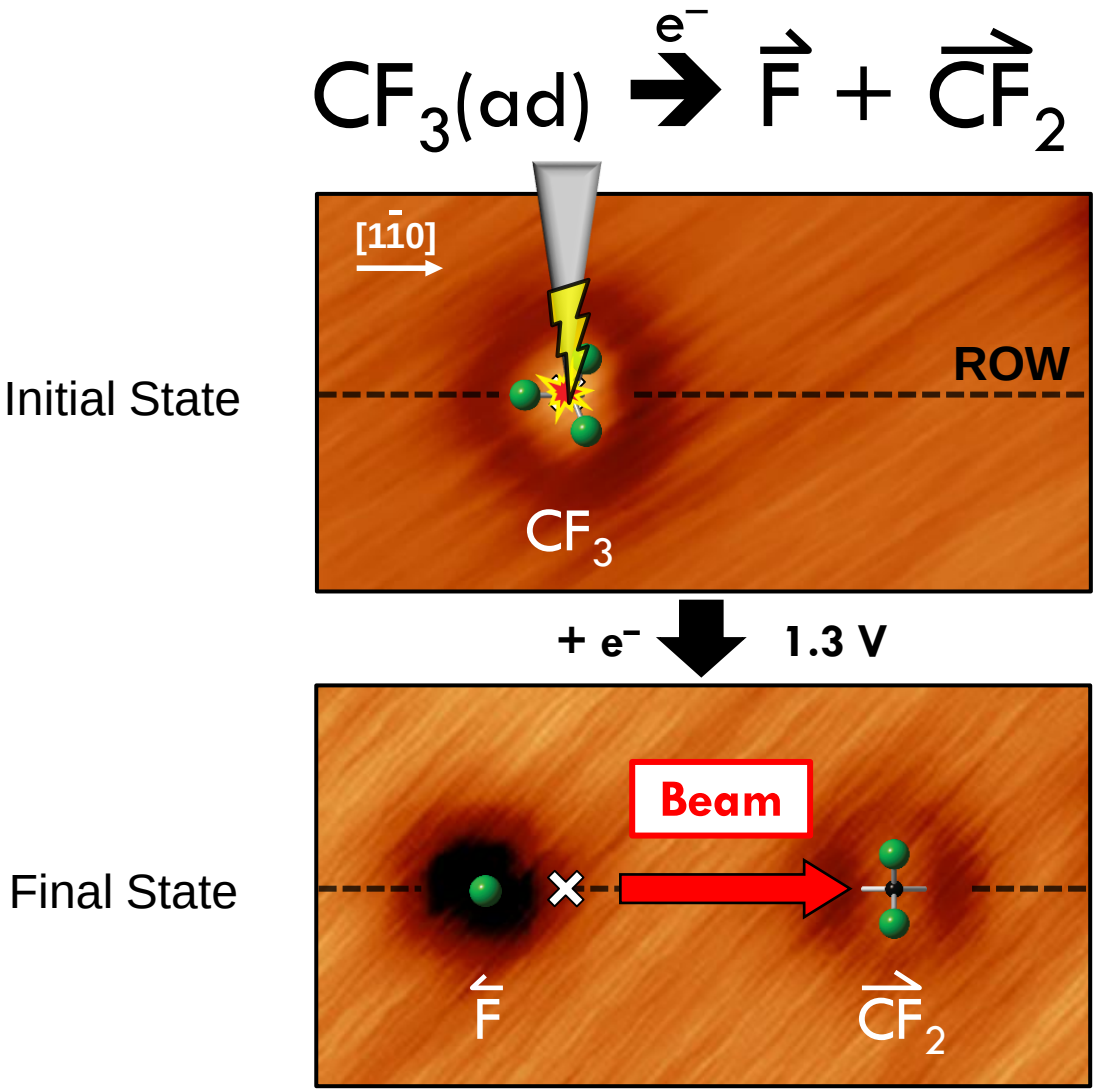
Simulation



Side view

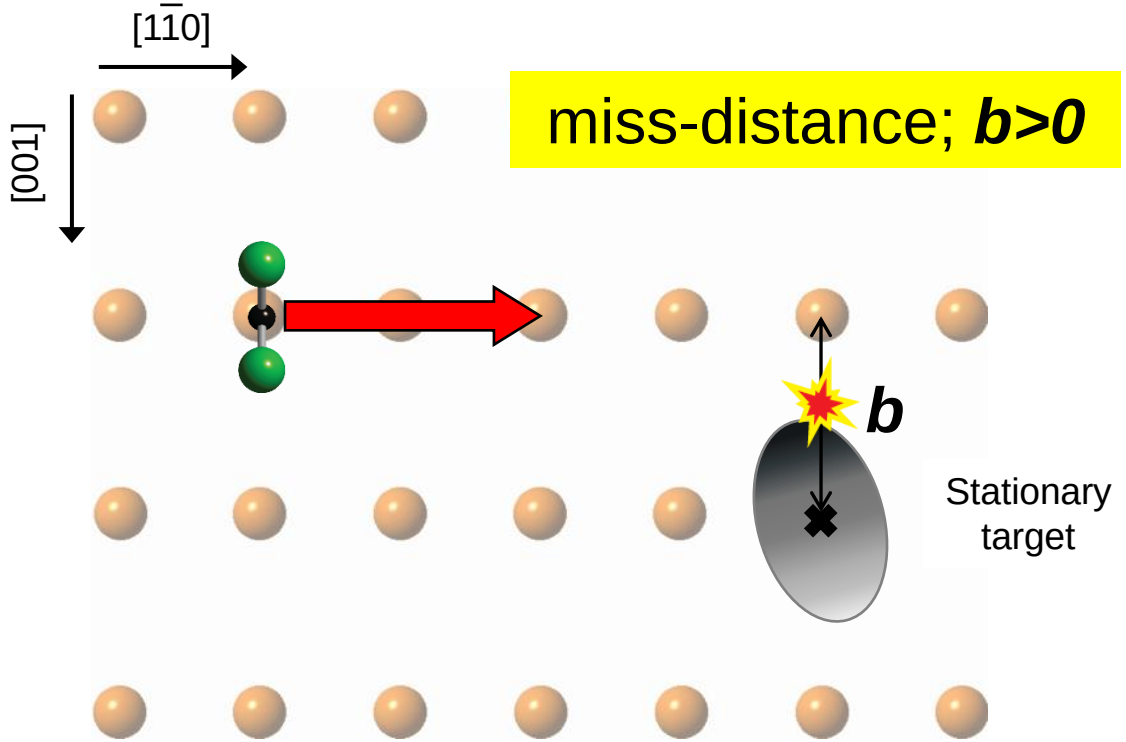


What is a ‘Surface-Molecular-Beam’ ?



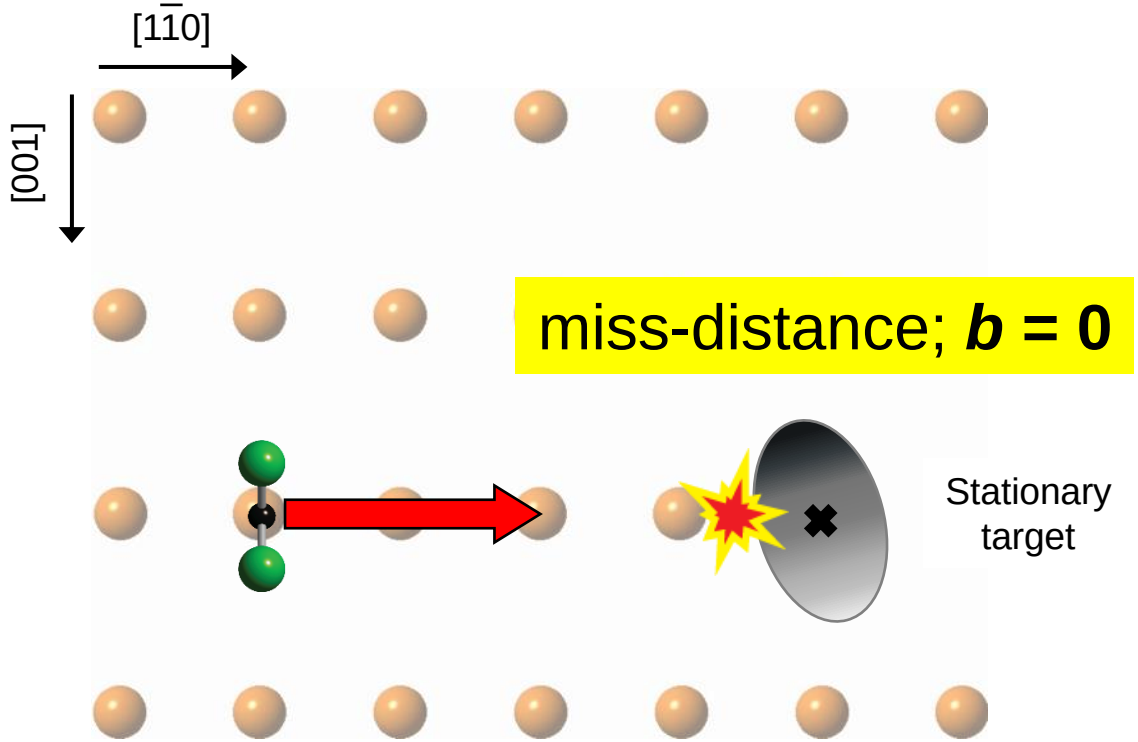
How to Direct a Collision:

Selecting Impact Parameter, ***b>0***



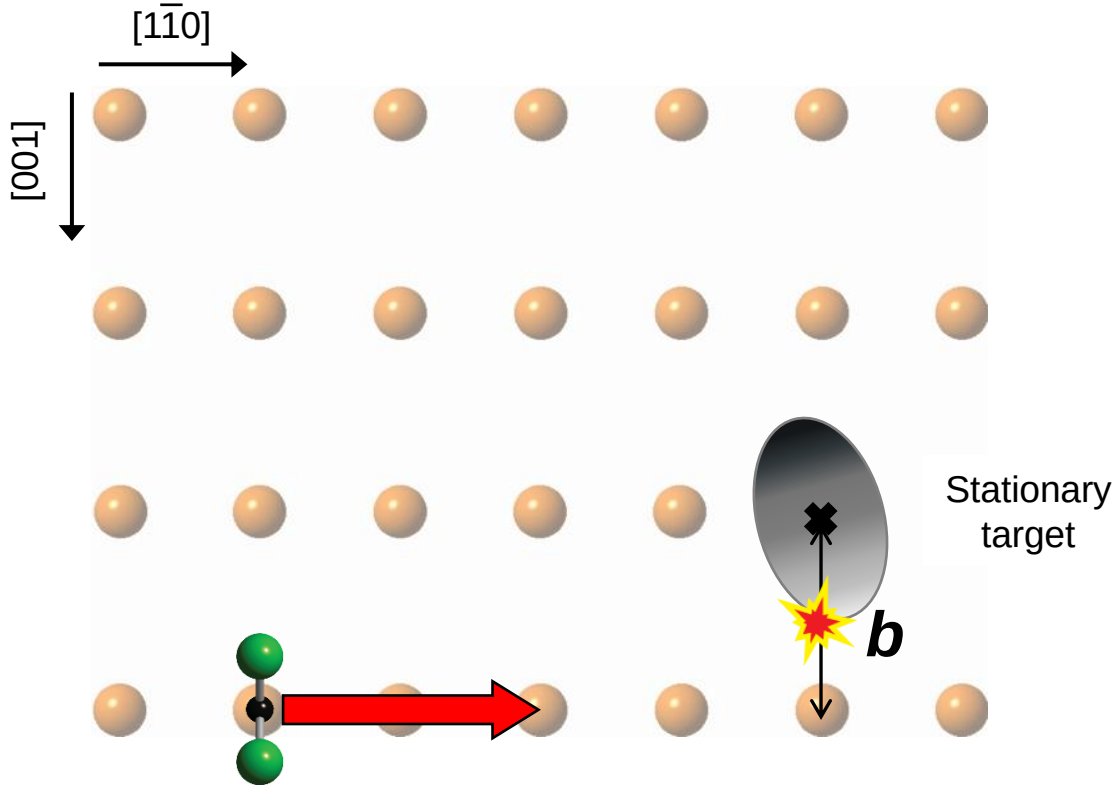
How to Direct a Collision:

Selecting Impact Parameter, ***b=0***



How to Direct a Collision:

Selecting Impact Parameter, ***b<0***

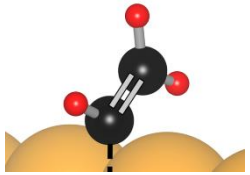


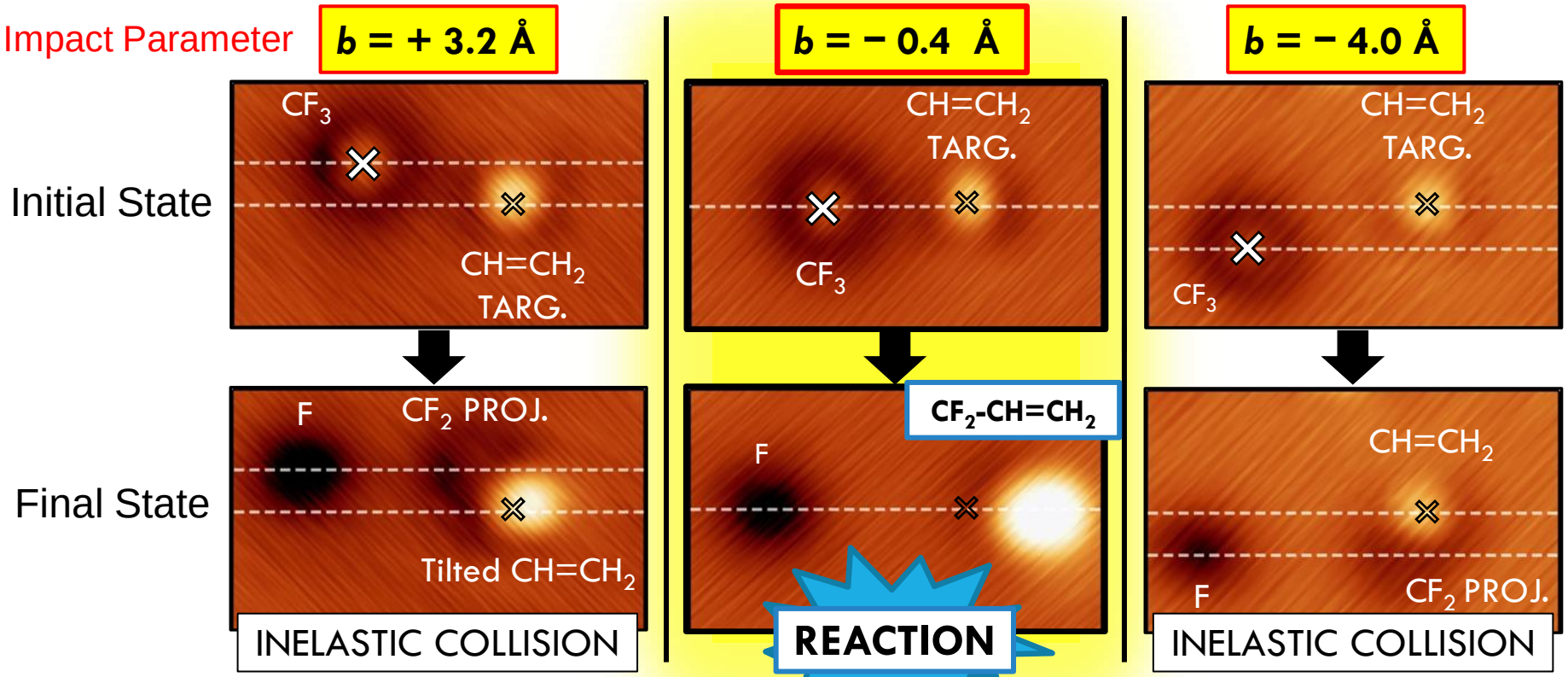
miss-distance; ***b<0***

EXPERIMENT

Example 1: Directed Collision with Vinyl (ad)

$\overrightarrow{CF_2}$ (projectile) + $CH{=}CH_2$(ad) (target)





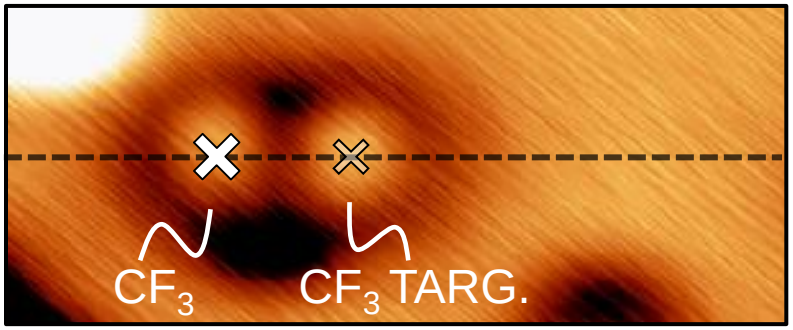
THREE OUTCOMES

EXPERIMENT

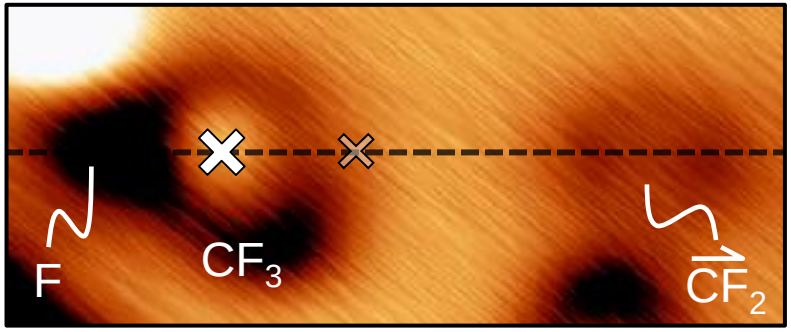
Example 2: Directed Collision with NEW Target, CF_3(ad)

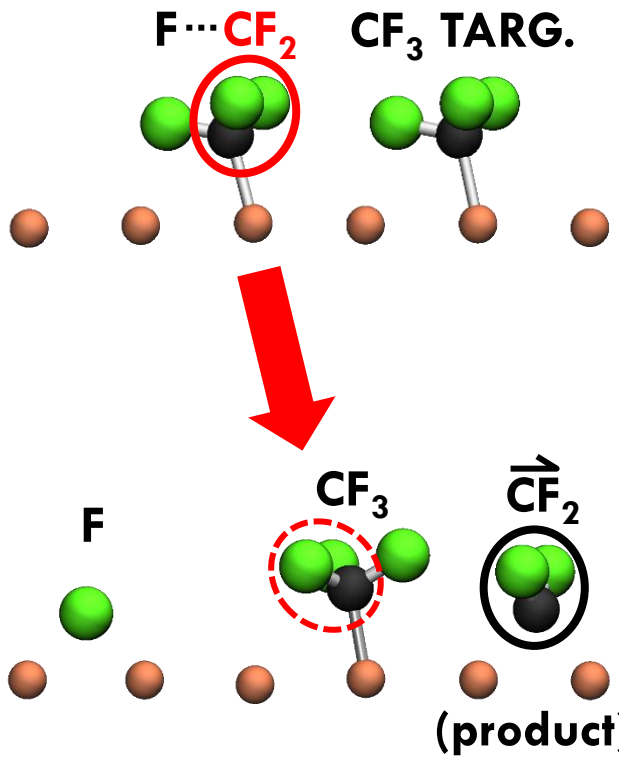
$\vec{CF}_2$ (projectile) + CF_3(ad) (target)

Initial State



Final State

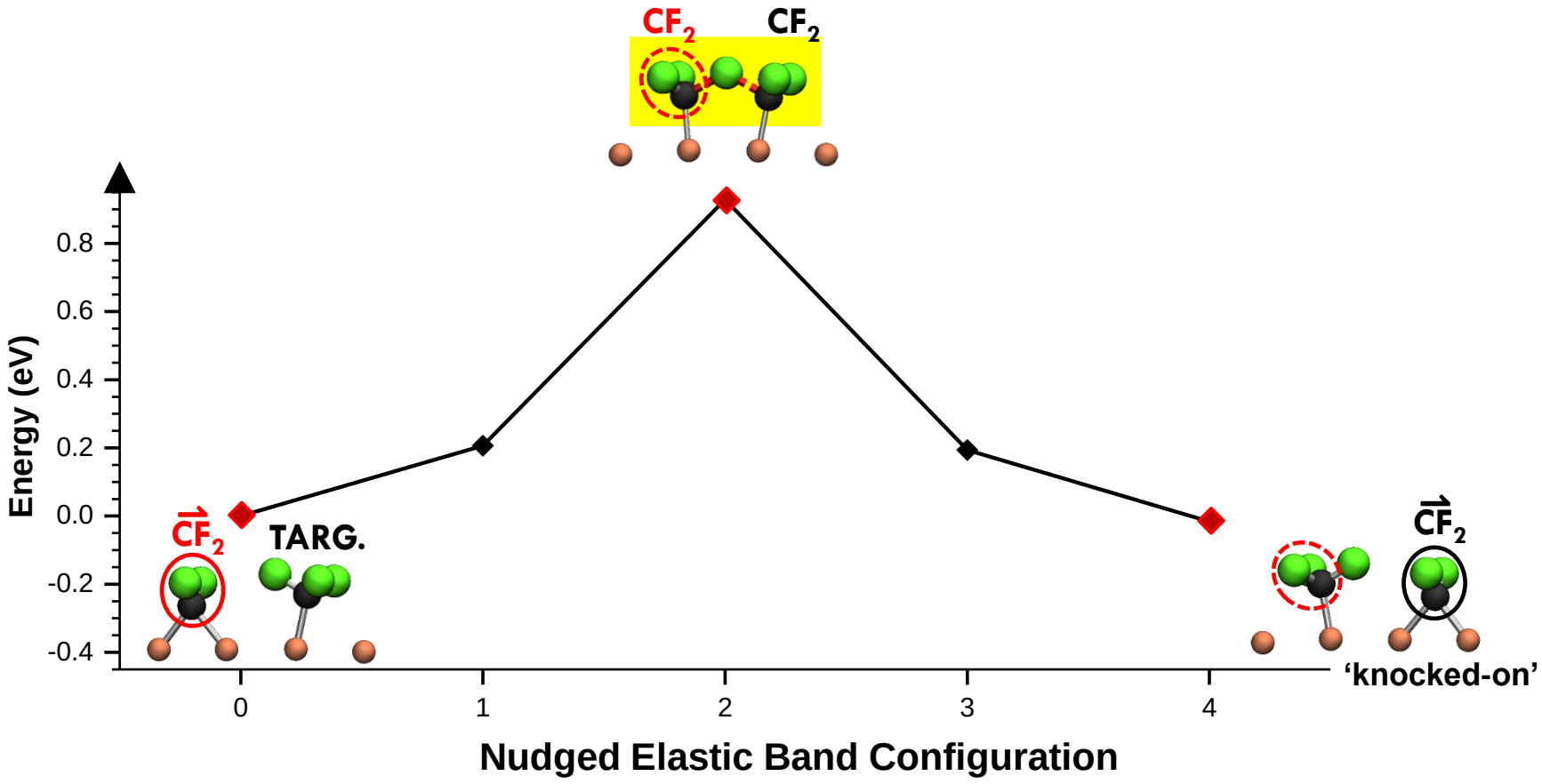




CF_2(projectile) 'knocks-on' CF_2(product)

EXPERIMENT
Example 2: Directed Collision with CF_3

Calculated Reaction Pathway, $\vec{CF}_2$ as Projectile

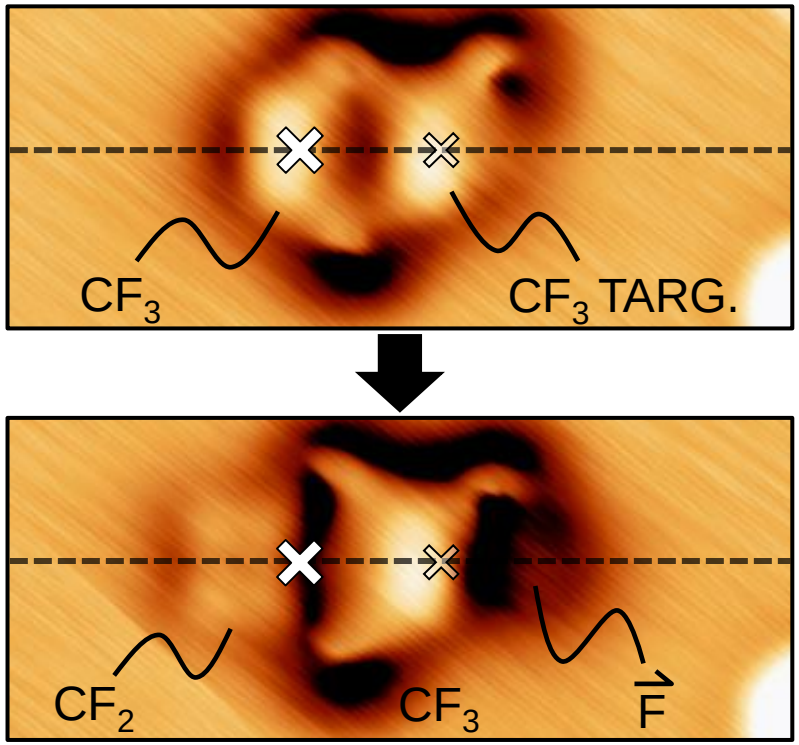


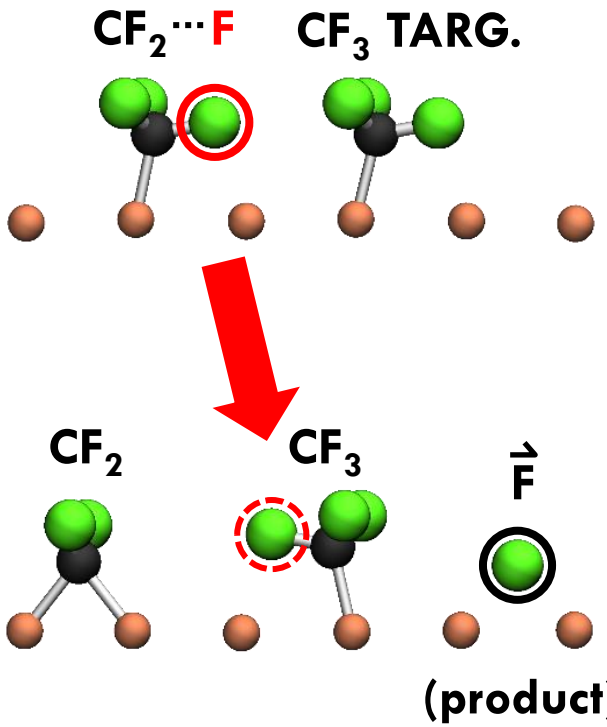
EXPERIMENT
Example 2: Directed Collision with CF_3

$\vec{F}$-atom (projectile) + CF_3(ad) (target)

Initial State

Final State

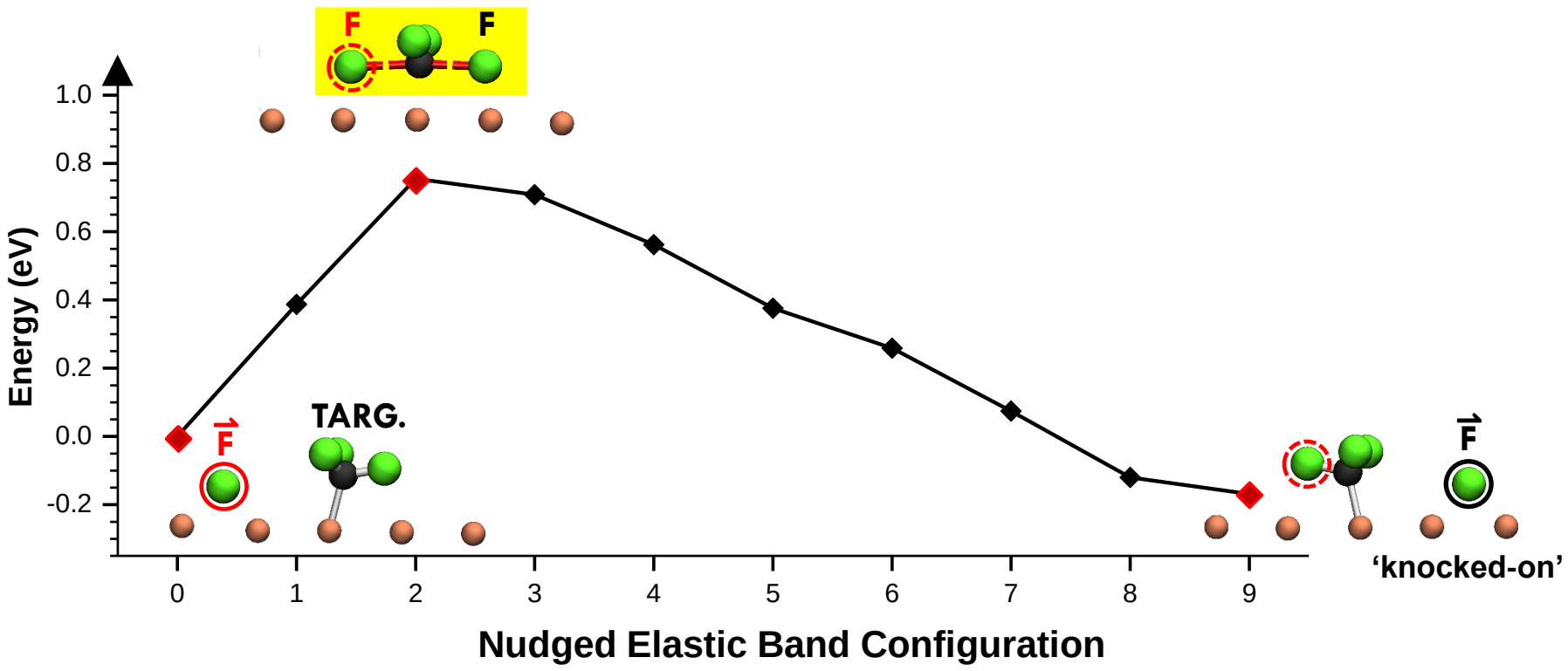




F-atom (projectile) 'knocks-on' F-atom (product)

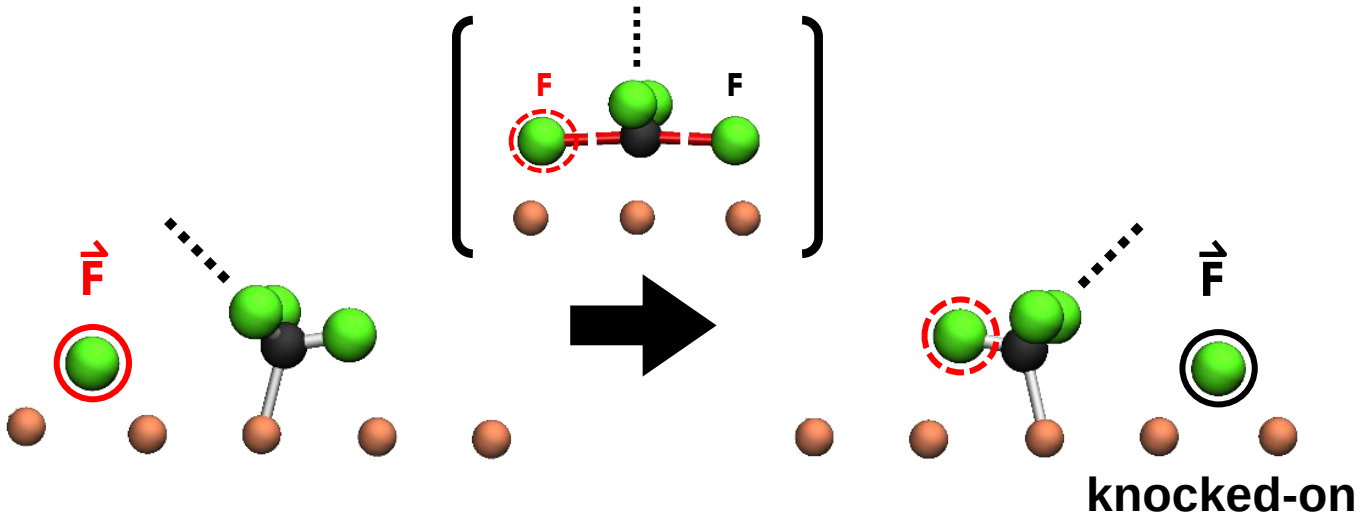
EXPERIMENT
Example 2: Directed Collision with CF_3

Calculated Reaction Pathway, $\vec{F}$-atom as Projectile



Conclusions

1) Surface-Molecular-Beam, Directed Collision
2) Choice of impact parameter; 'Reaction' or 'Inelastic'
3) 'Knock-on'; $\vec{CF}_2$ or $\vec{F}$ with umbrella inversion



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