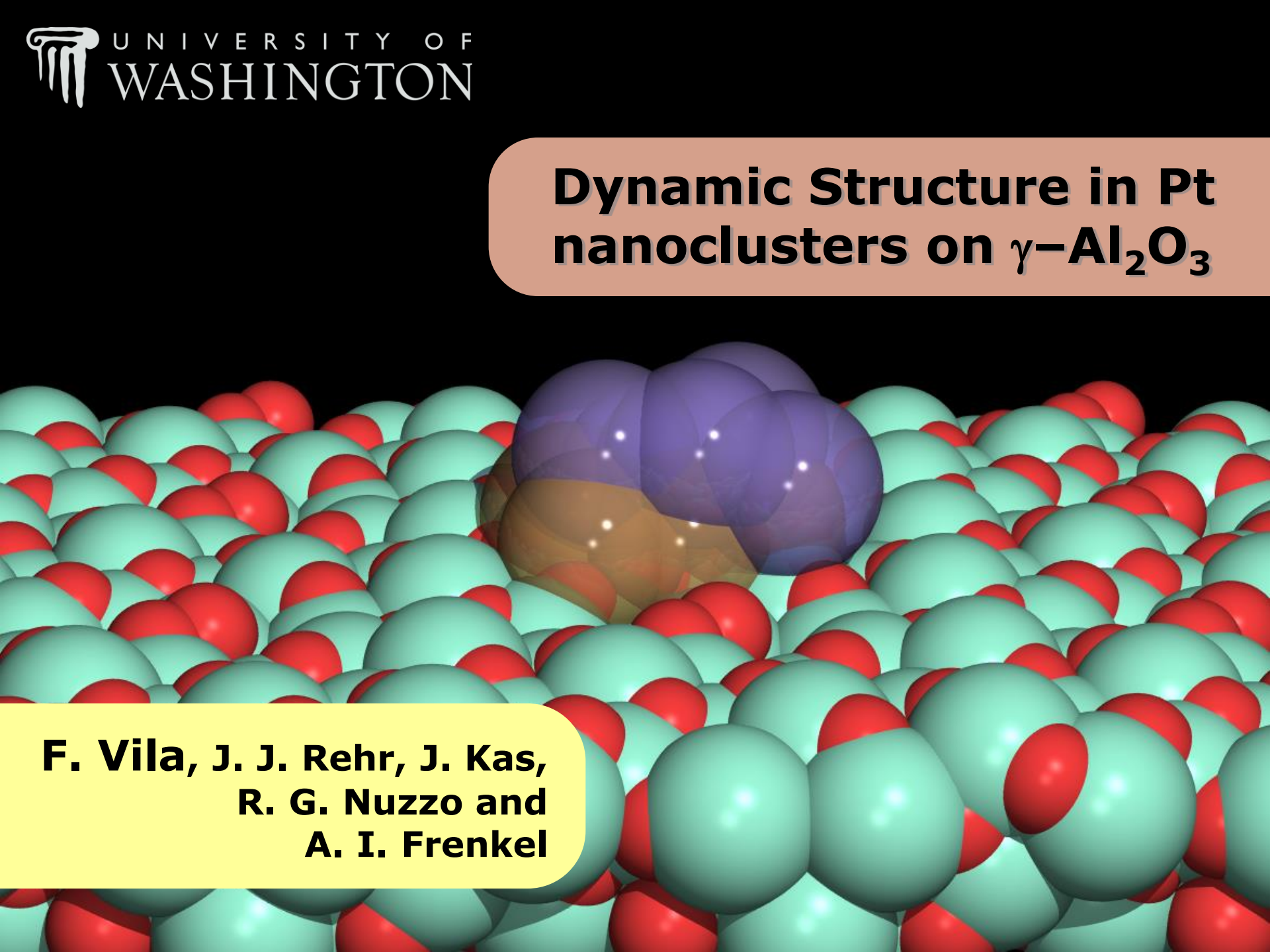


# Dynamic Structure in Pt nanoclusters on $\gamma\text{-Al}_2\text{O}_3$



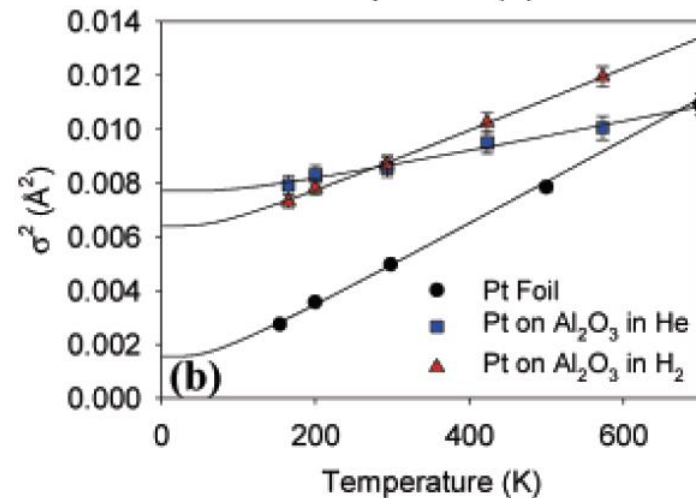
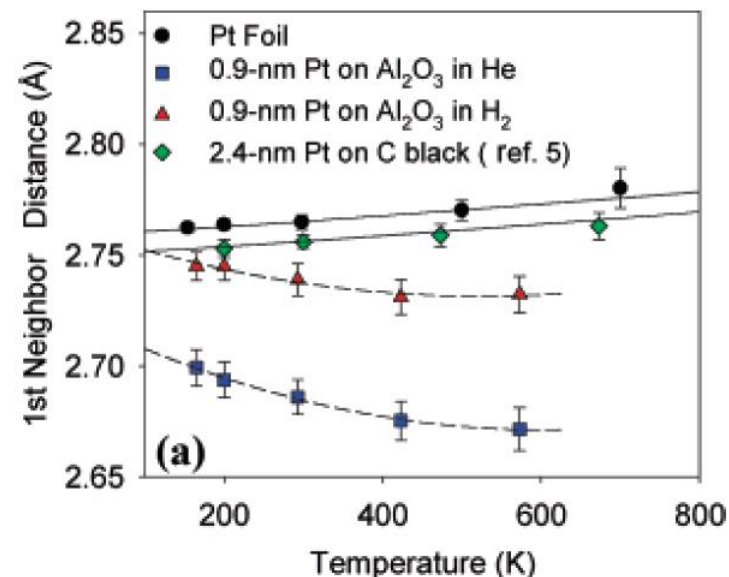
**F. Vila, J. J. Rehr, J. Kas,  
R. G. Nuzzo and  
A. I. Frenkel**

Pt-Pt bond **expansion**  
going from He to H<sub>2</sub>  
atmosphere ①

Pt-Pt bond **negative**  
**thermal expansion** ②

High Pt-Pt **disorder** ③

**Increased intensity**  
and **redshift** of XANES  
with increasing T ④

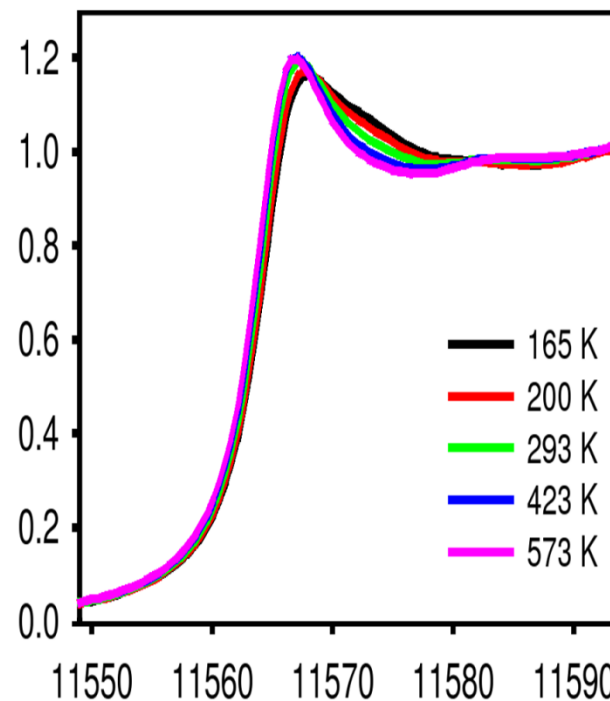


Pt-Pt bond **expansion**  
going from He to H<sub>2</sub>  
atmosphere ①

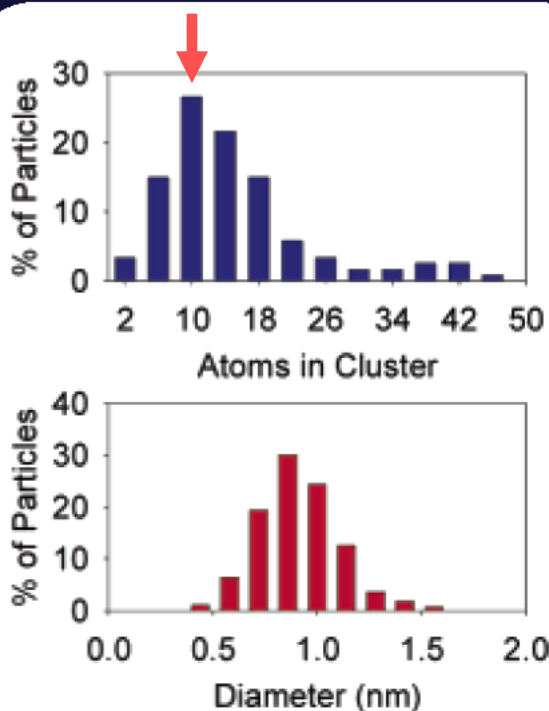
Pt-Pt bond **negative**  
**thermal expansion** ②

High Pt-Pt **disorder** ③

**Increased intensity**  
and **redshift** of XANES  
with increasing T ④



**Study prototypical  
Pt<sub>10</sub> cluster  
on [110] surface  
of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>**



## DFT/MD

**VASP**

**PBE Functional**

**396 eV Cutoff**

**3 fs Step**

**3 ps Equilibration**

**5 ps Runs (3)**

**165 K & 573 K**

## XANES

**FEFF8**

**Full Multiple Scattering**

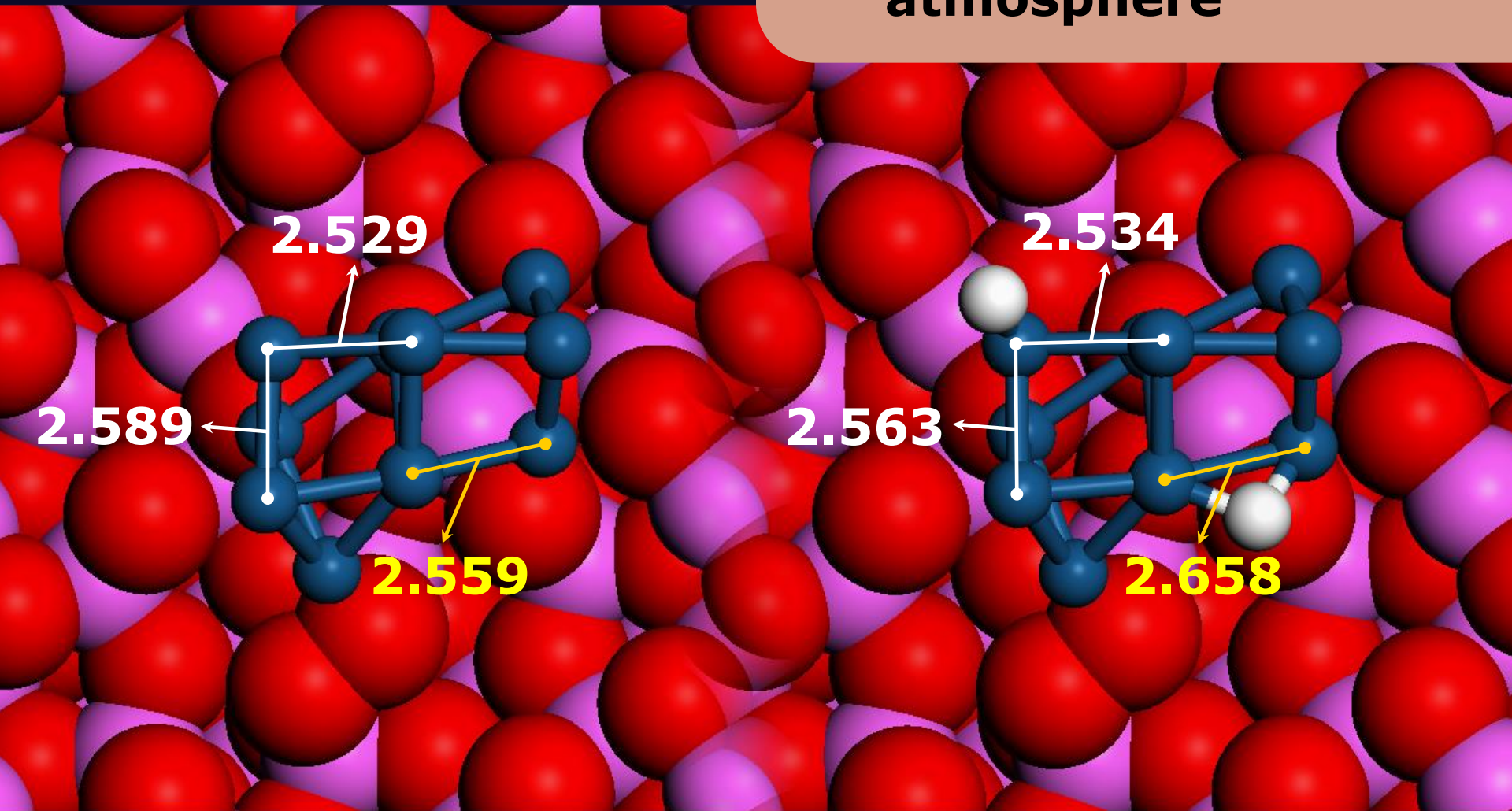
**32 Configurations from MD**

**7 Å Clusters (~150 atoms)**

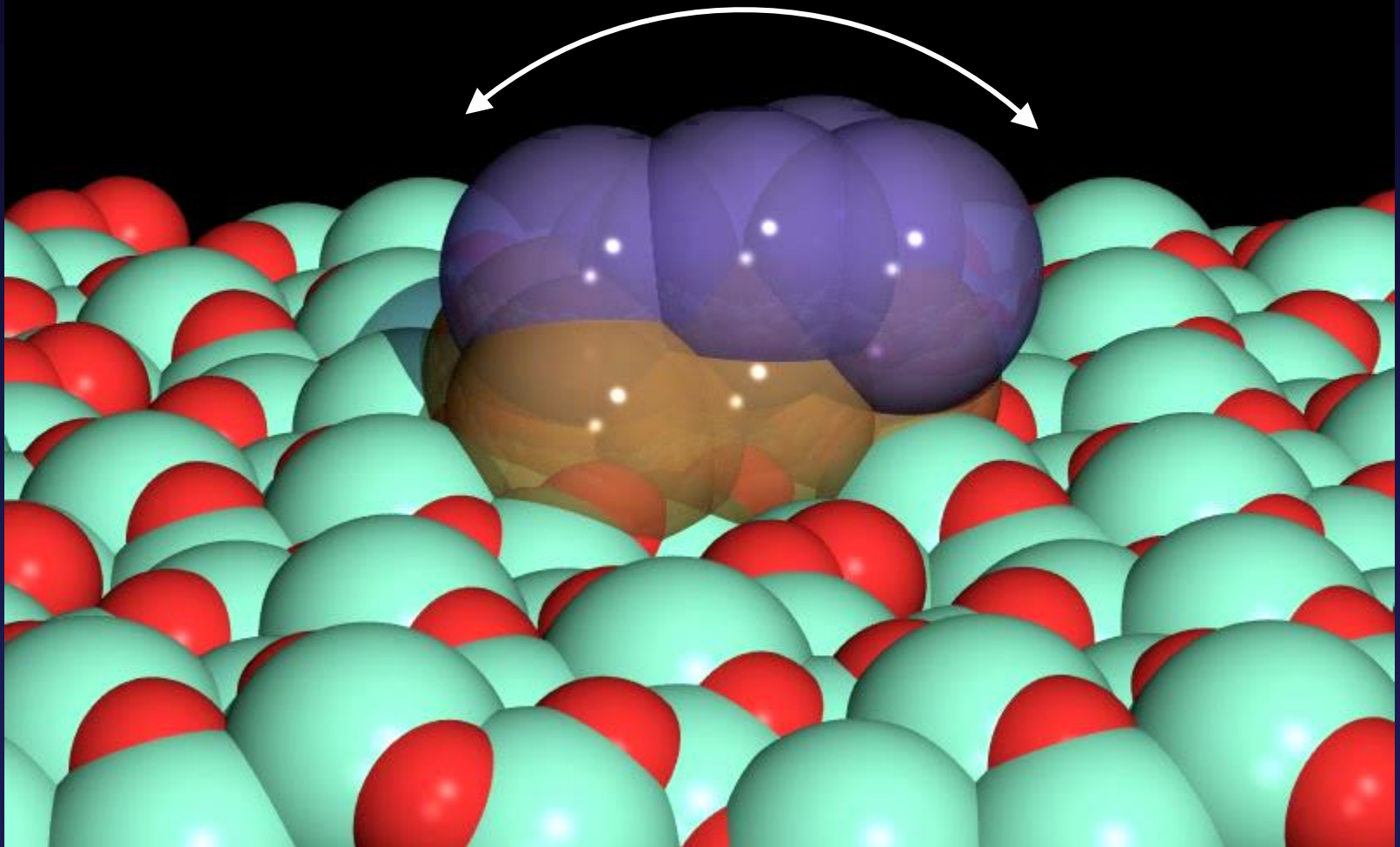


1

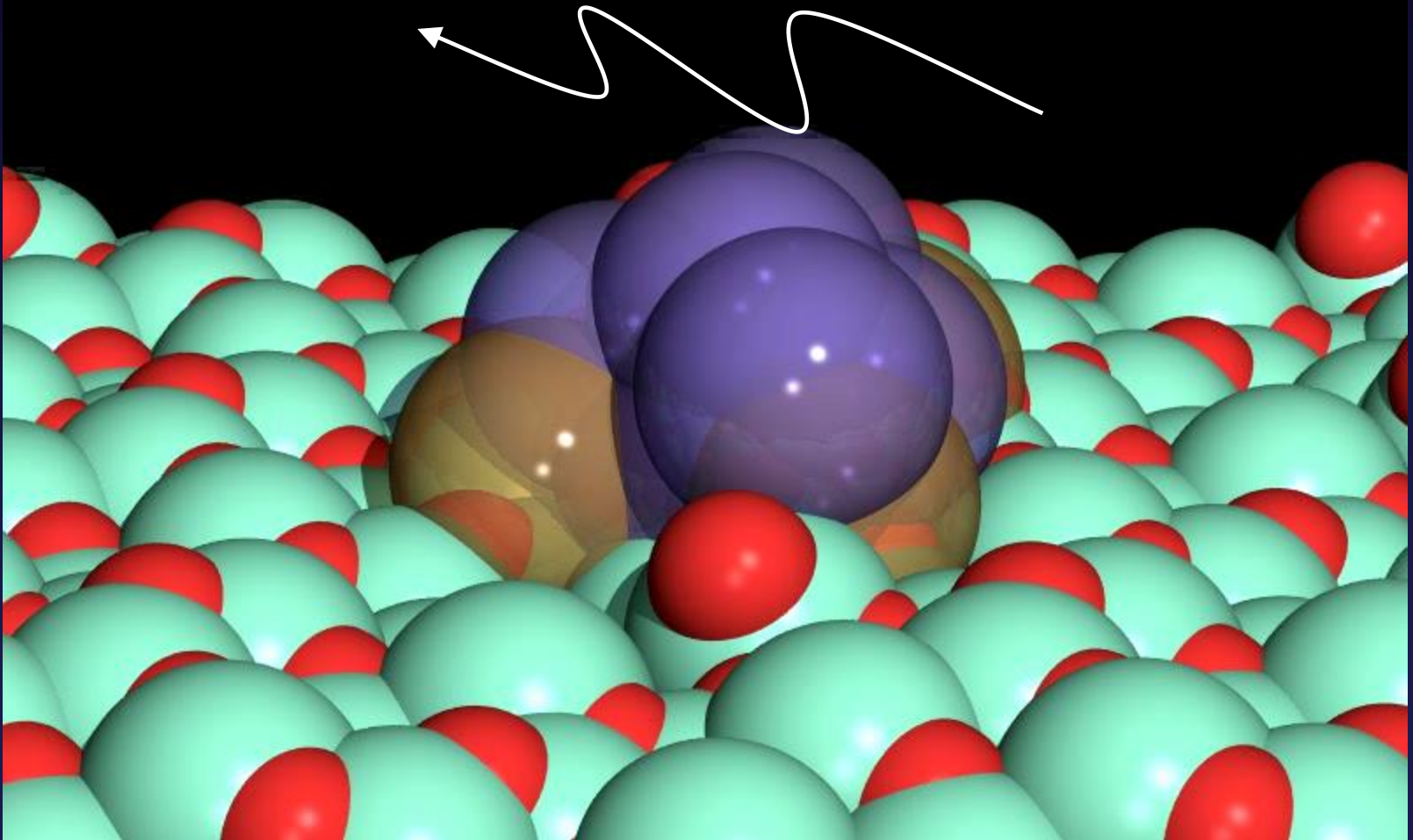
# Bond expansion in H<sub>2</sub> atmosphere



**Librational Motion**

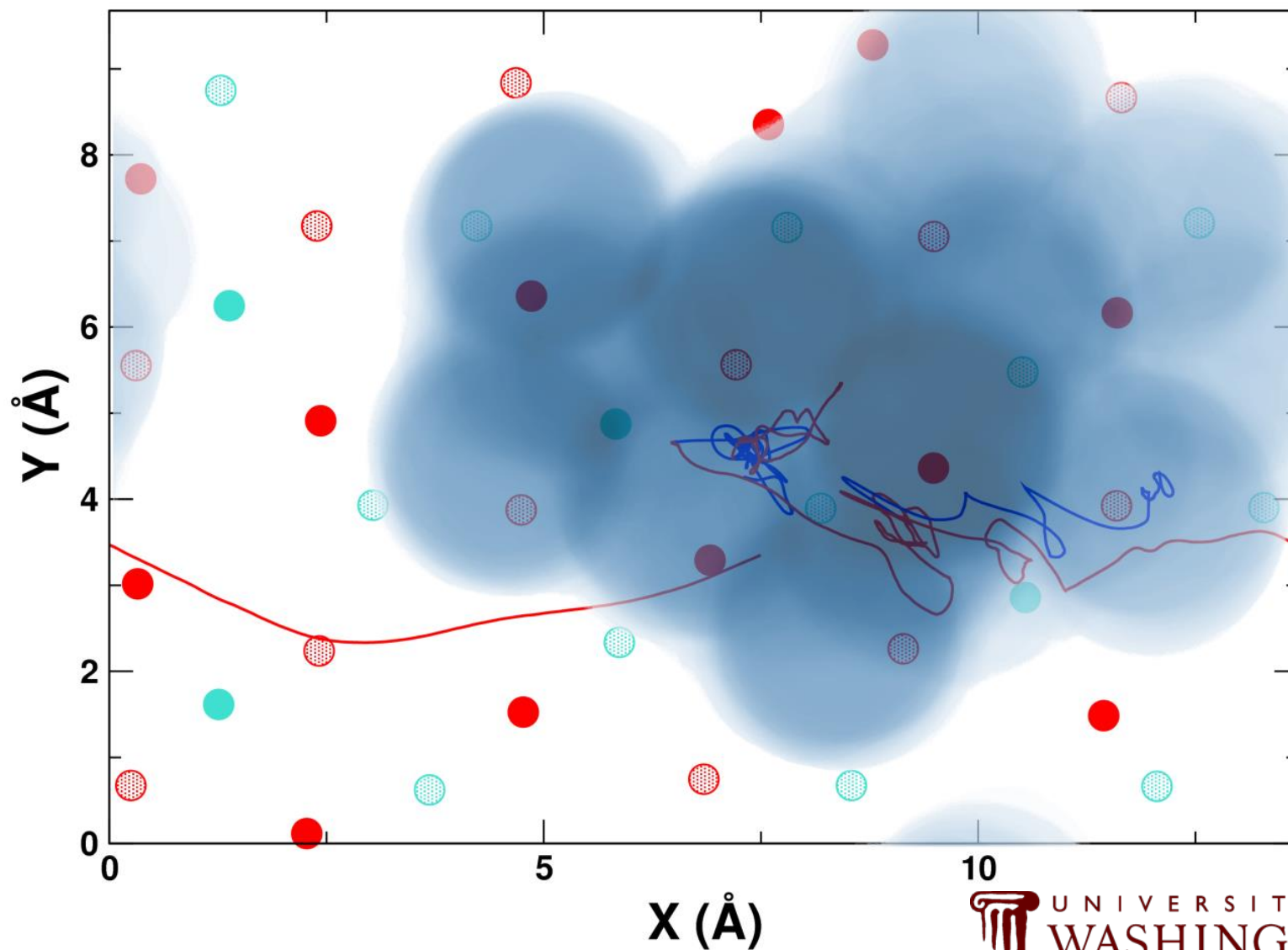


**Brownian-like Motion**



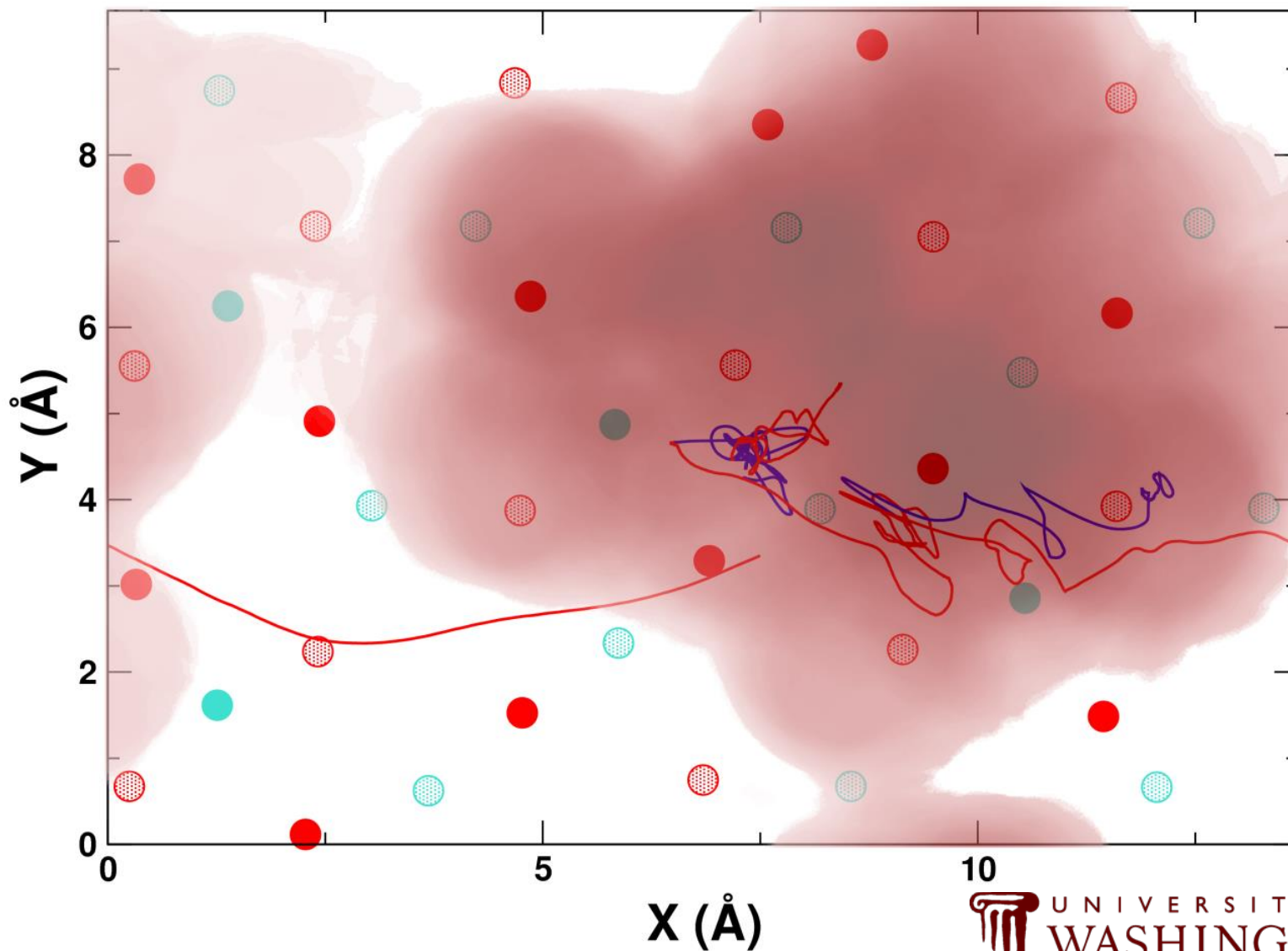


# Cluster footprint @ 165 K

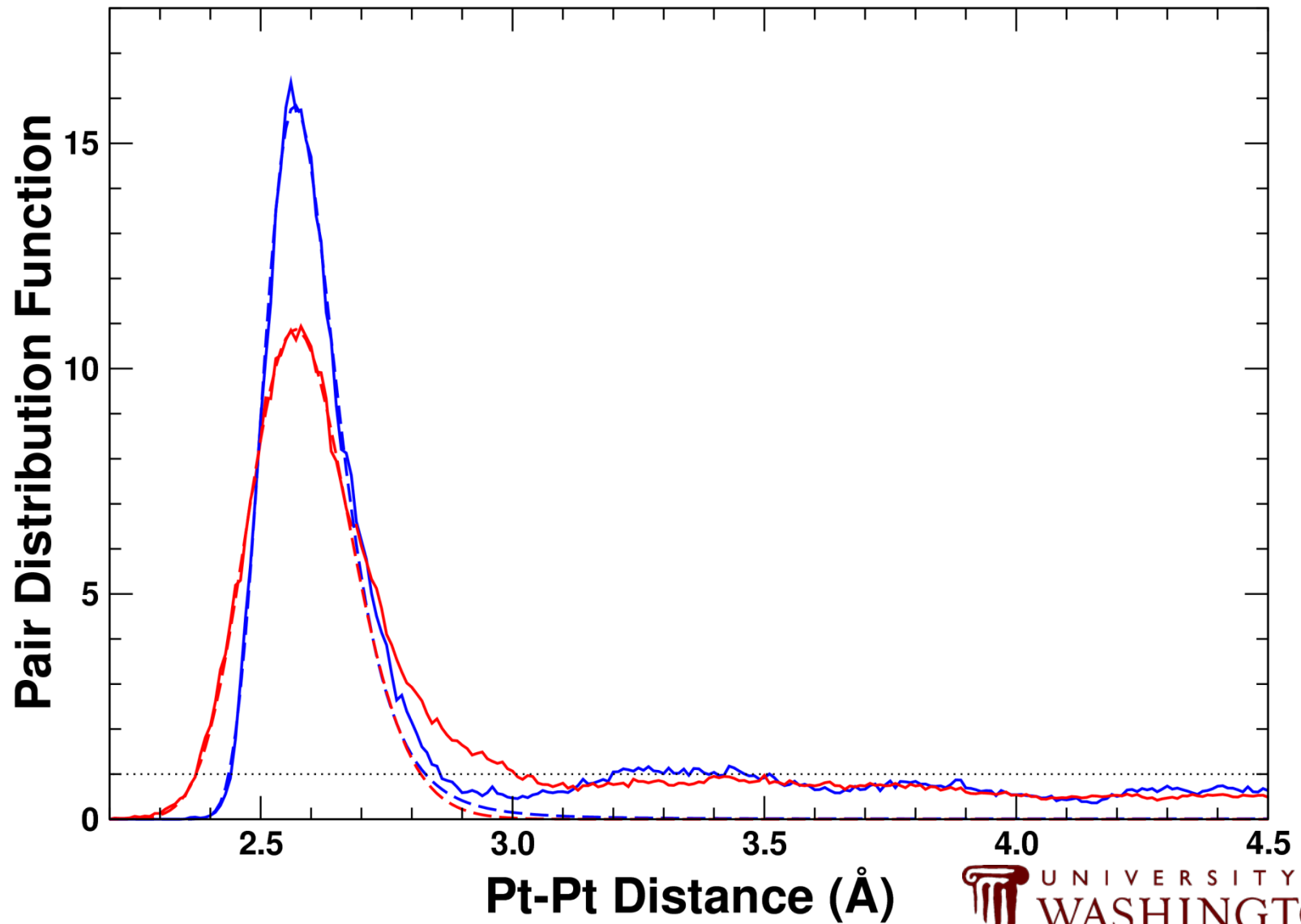




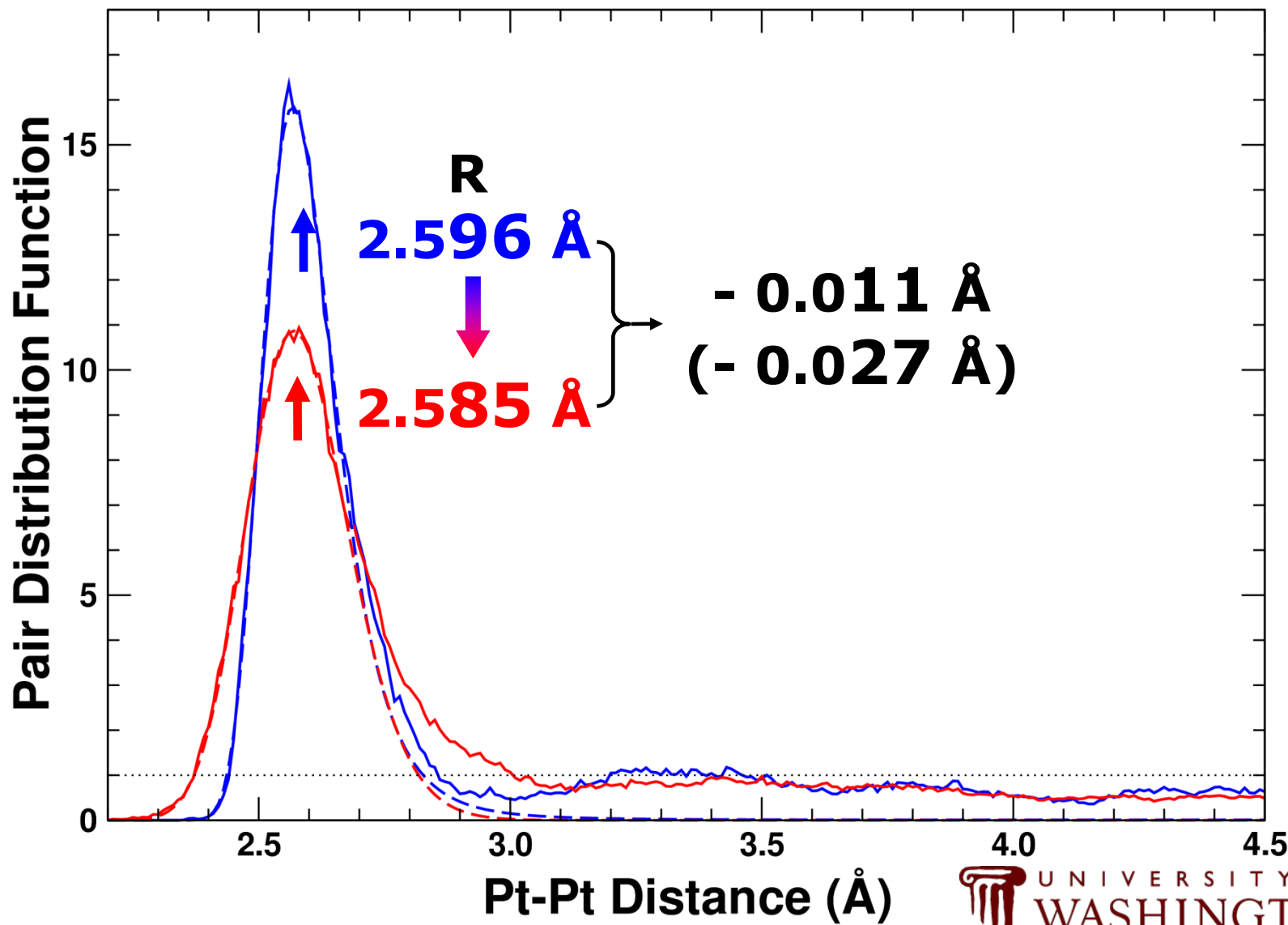
# Cluster footprint @ 573 K



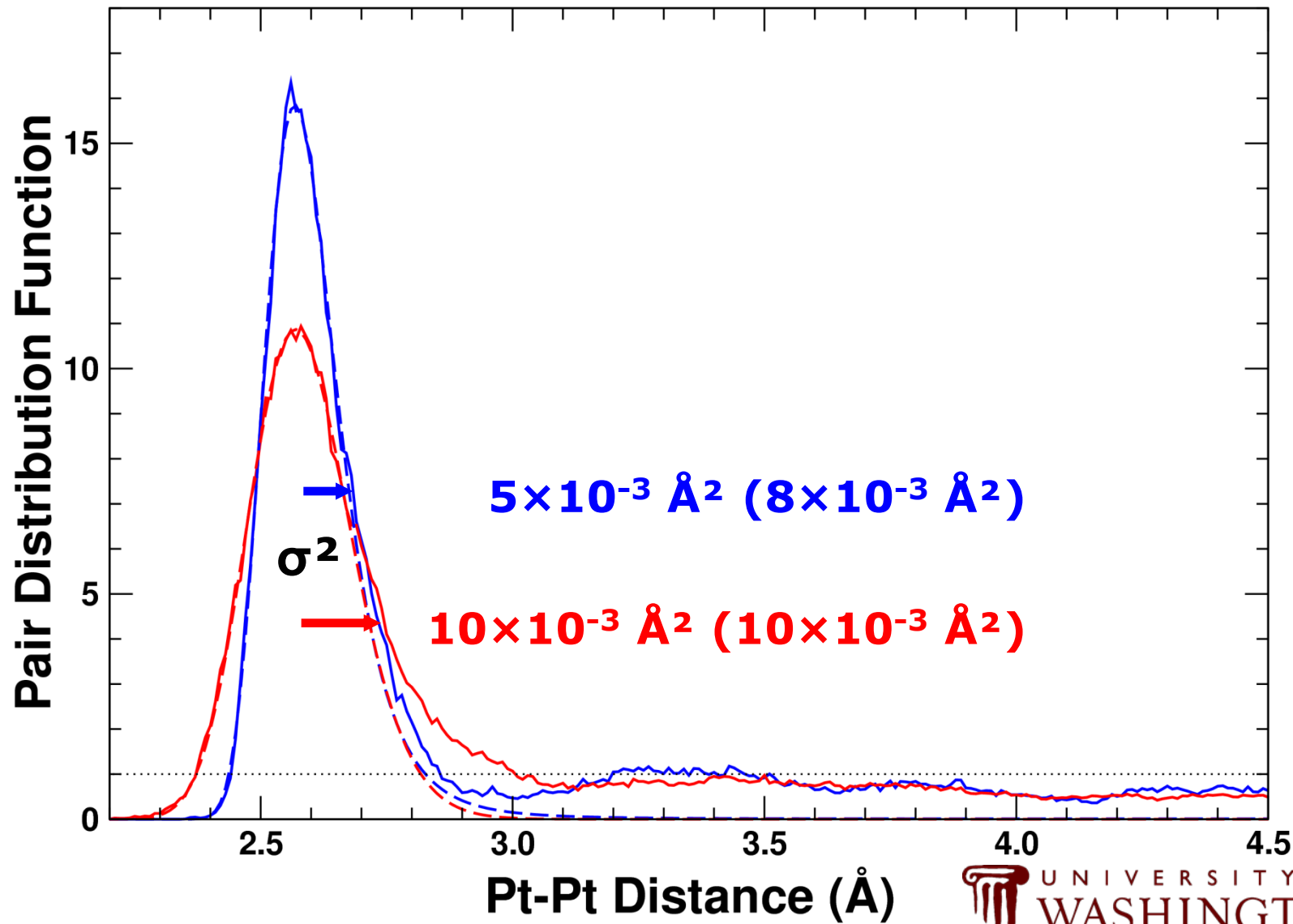
# Pt-Pt Pair Distribution Function



## ② Negative Thermal Expansion

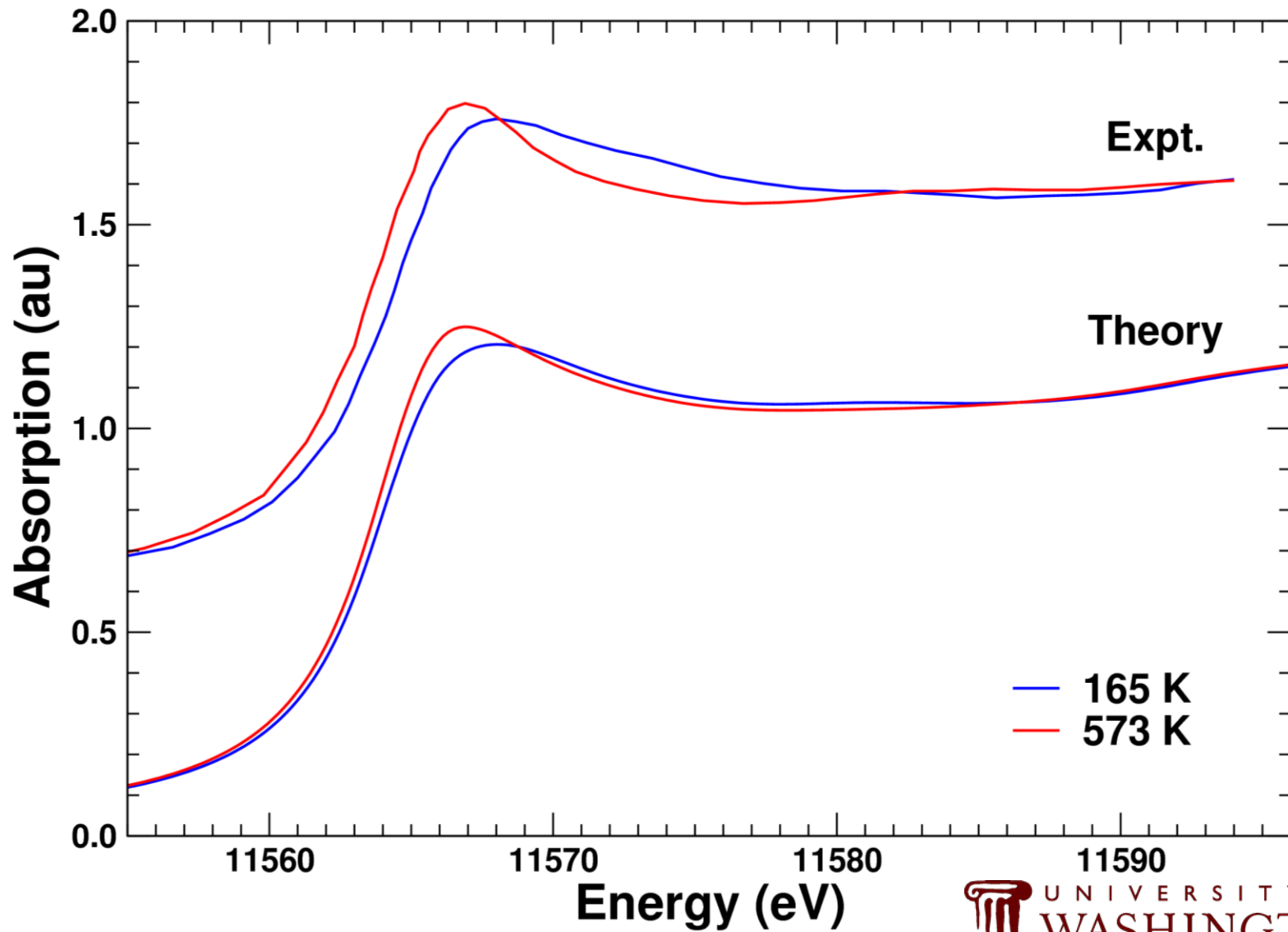


### 3 High Pt-Pt Disorder

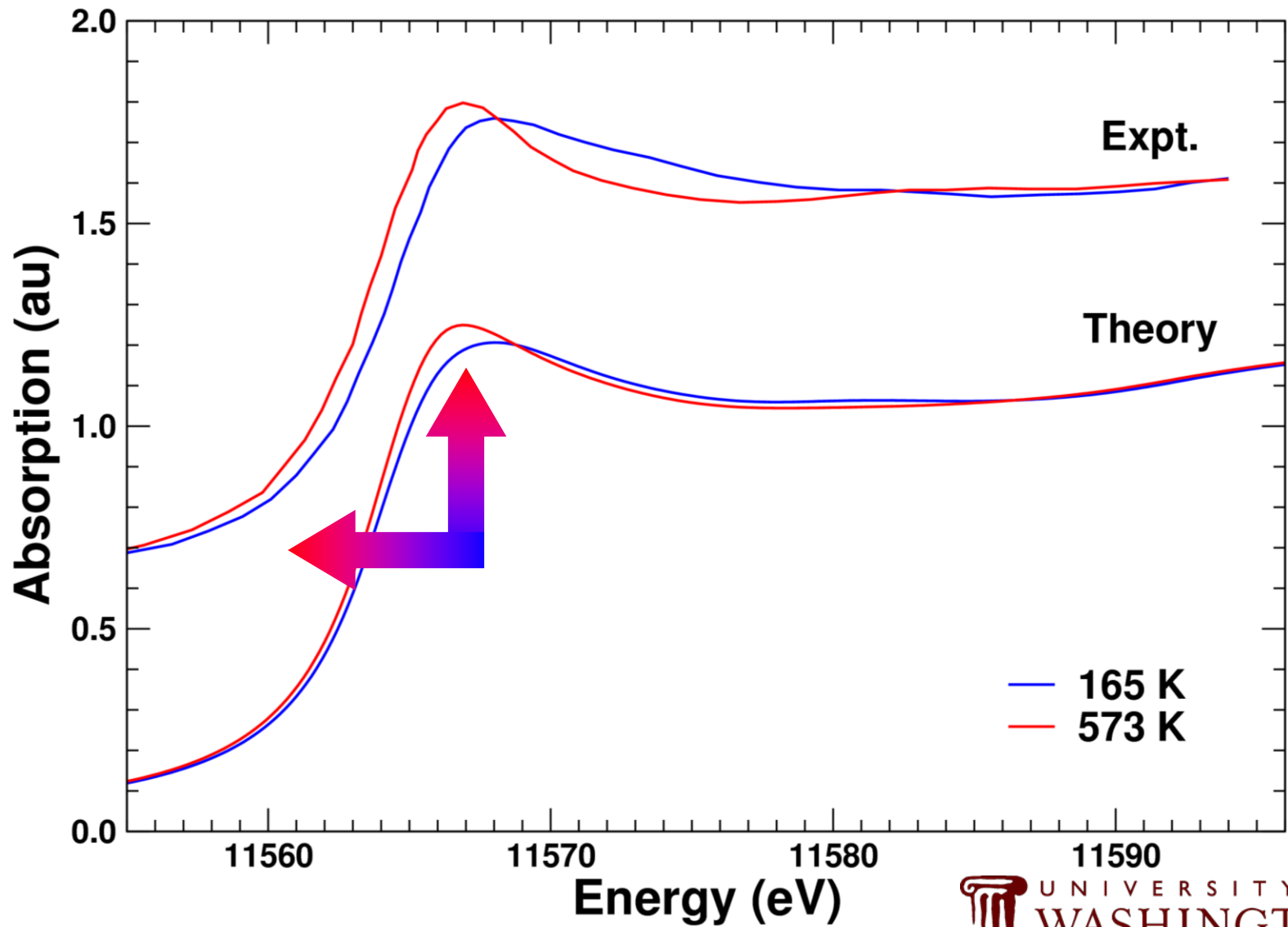




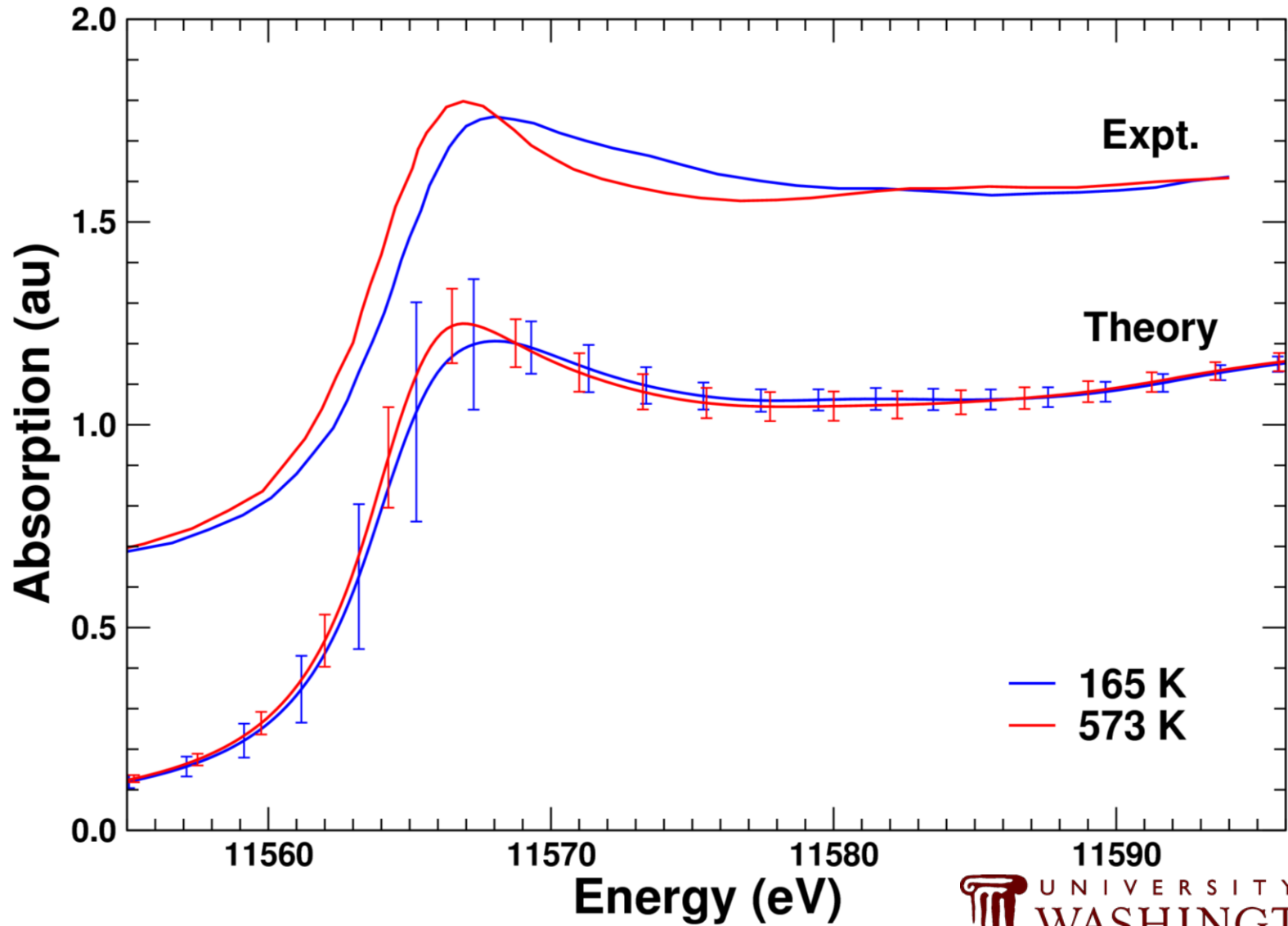
# Pt L<sub>3</sub> XANES



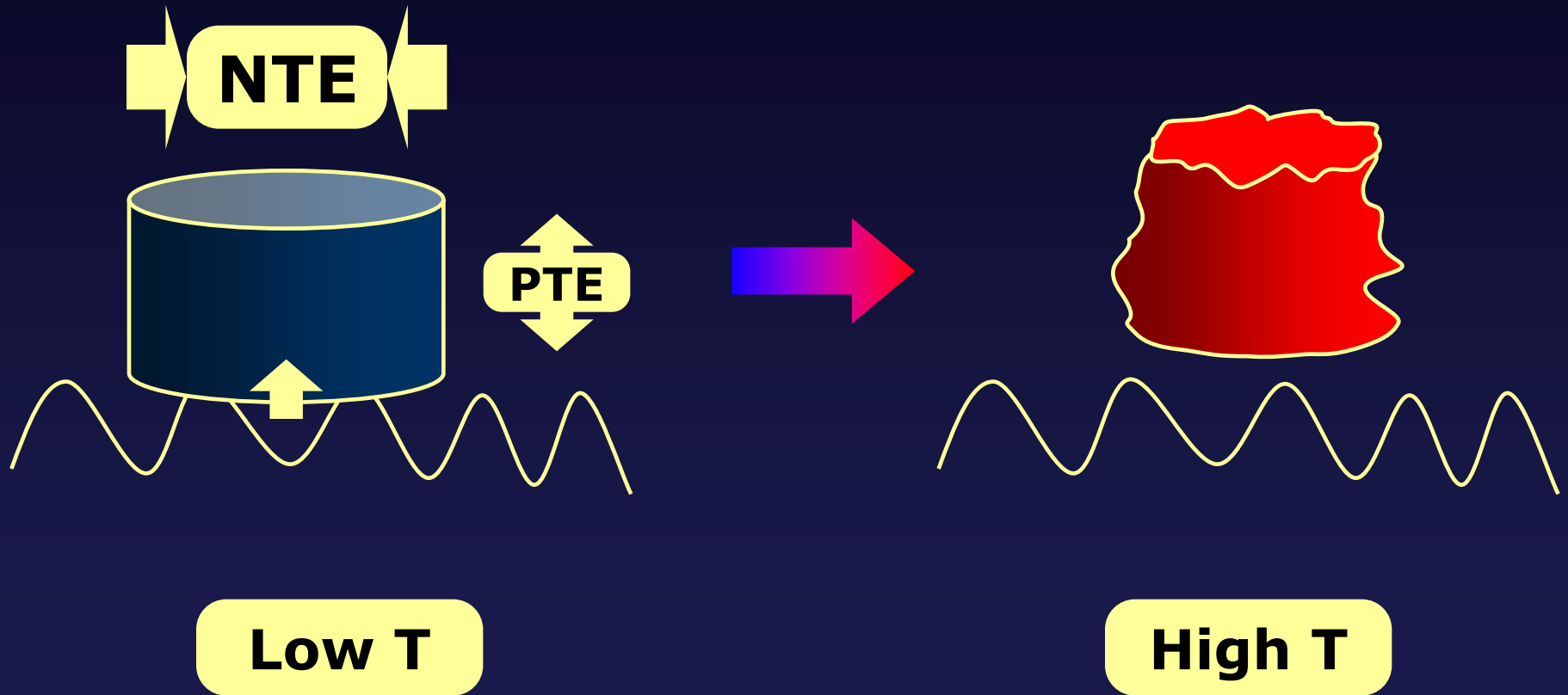
## ④ Increased intensity and redshift at high T



# ⑤ Increased intensity and redshift at high T



# A Simple Model





**Found agreement with all  
experimental observations:  
structural and spectroscopic**

**1**

**Discovered some unusual  
dynamical behavior:  
Librational and Brownian-like  
motion**

**2**

**Possible implications in catalysis:  
Activity affected by cluster  
mobility?**

**3**

# Dynamic Structure in Pt nanoclusters on $\gamma\text{-Al}_2\text{O}_3$



Thank you...