

# Isomerization Mechanism and IR Spectra of Strongly Hydrogen Bonded HCl-Water Nanoclusters

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# Motivations and Methods

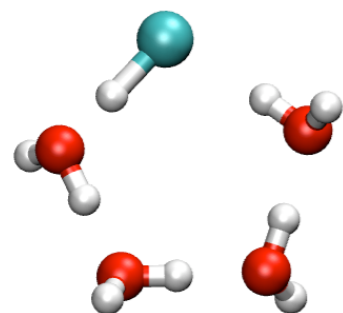
*TARGET:*

Understanding the acid dissociation of  $\text{HCl}(\text{H}_2\text{O})_4$  clusters, the isomerization mechanism and relating them to experimental IR spectra.

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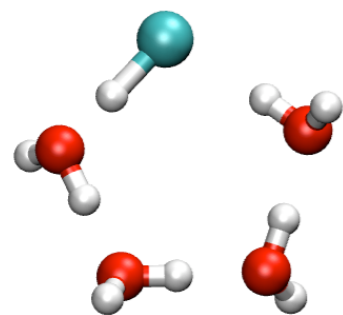


Undissociated  
2.7 kcal/mol

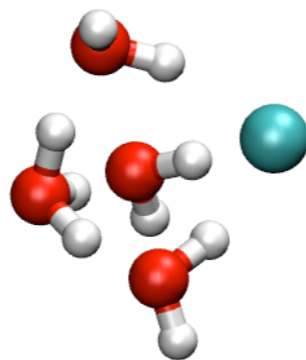
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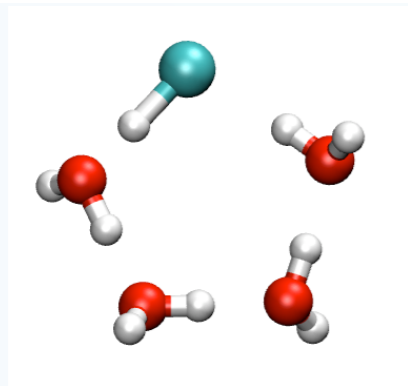


Dissociated  
0.0 kcal/mol

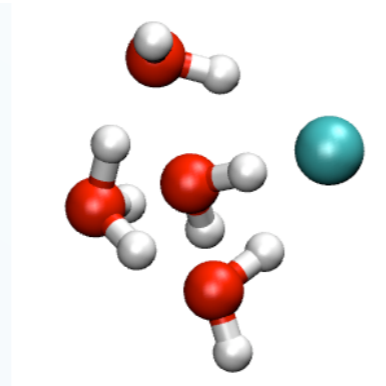
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## MACHINERY:

Ab initio MD simulations with BLYP/PW + Troullier-Martins pseudos (cutoff 70 Ry).

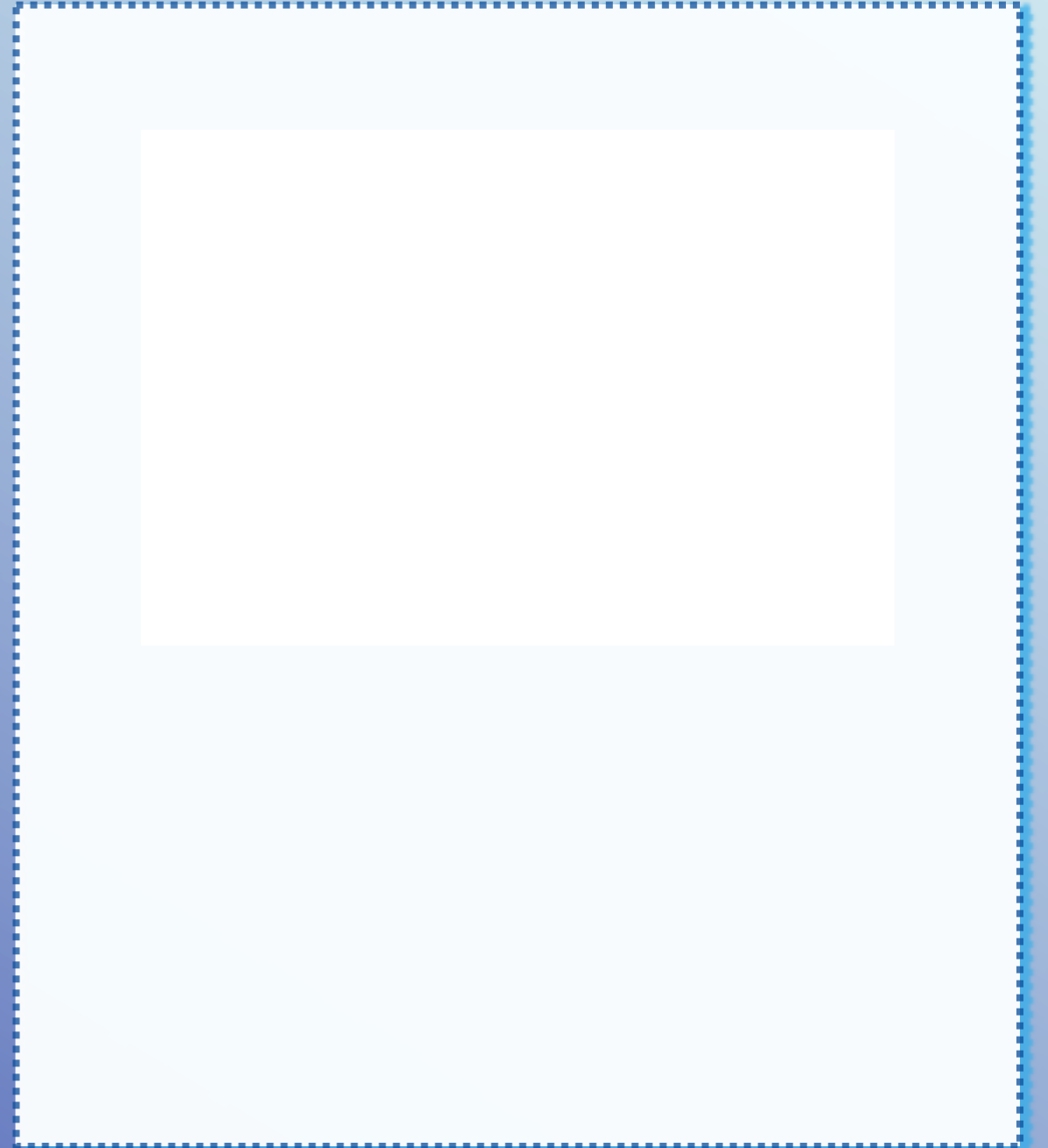
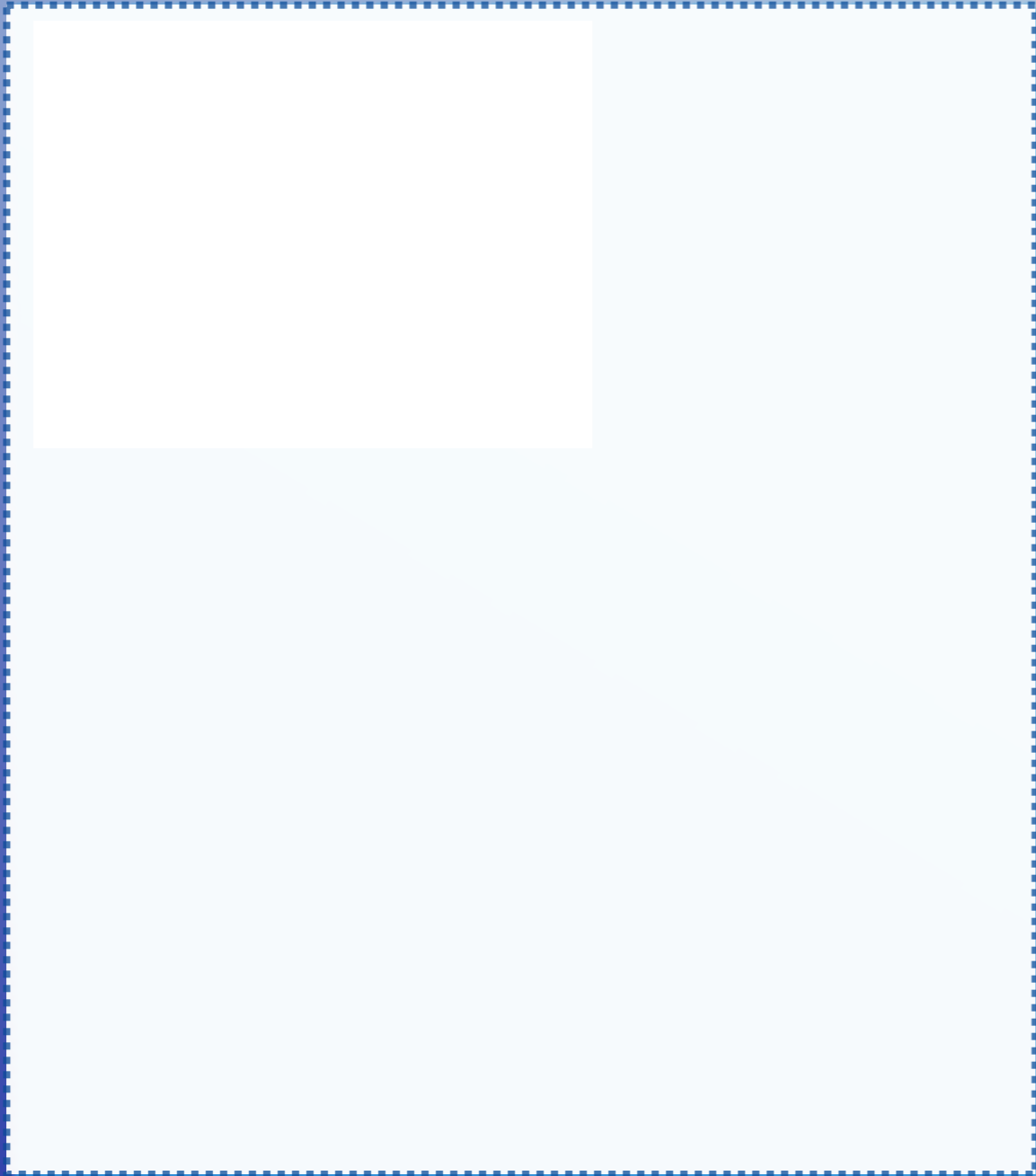
Born-Oppenheimer MD has been used for dynamics (spectra).

Car-Parrinello Metadynamics has been used for exploring the free energy surface. The collective variables being (i) the Cl-O coordination number

$$CN_{\text{Cl-O}} = \sum_{j=1}^{n_{\text{O}}} \left[ \frac{1 - \left( \frac{r_{\text{Cl-O}_j}}{r_0} \right)^m}{1 - \left( \frac{r_{\text{Cl-O}_j}}{r_0} \right)^n} \right]$$

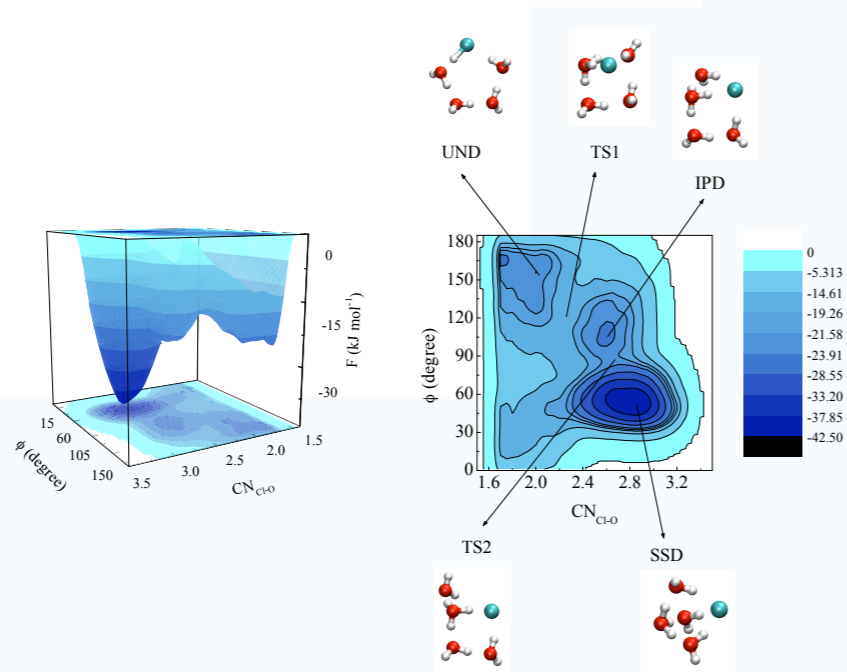
and (ii) the O-O-O-O dihedral angle  $\phi$

# Results and Conclusions



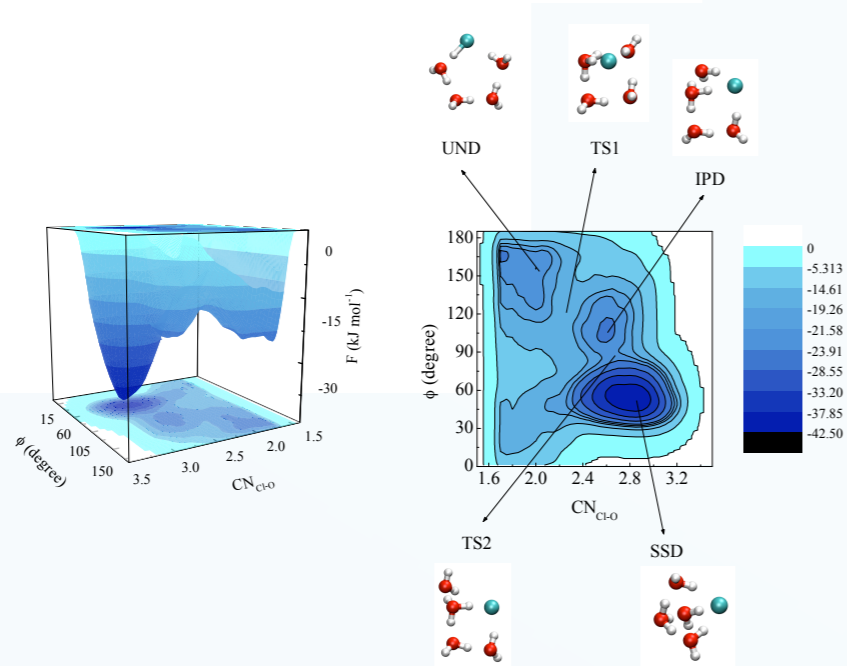
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## Free Energy Surface:

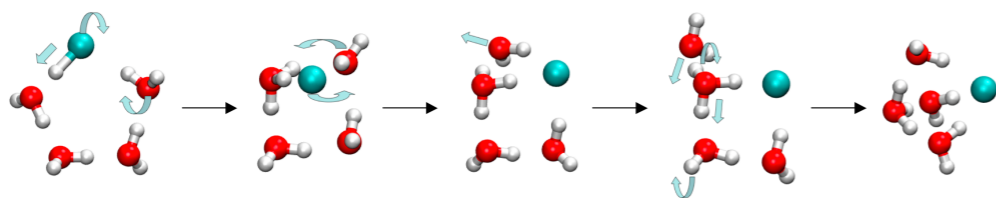


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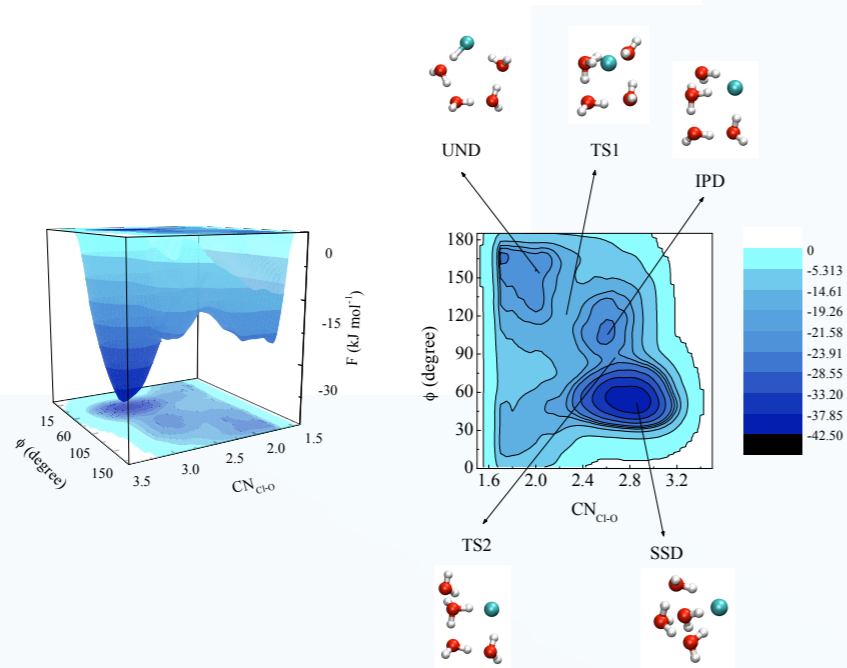
## The Mechanism:



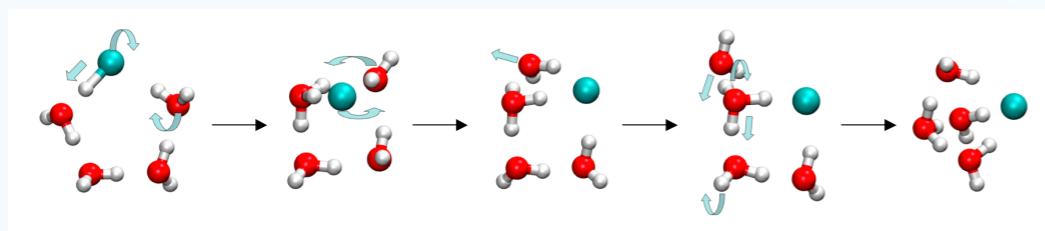


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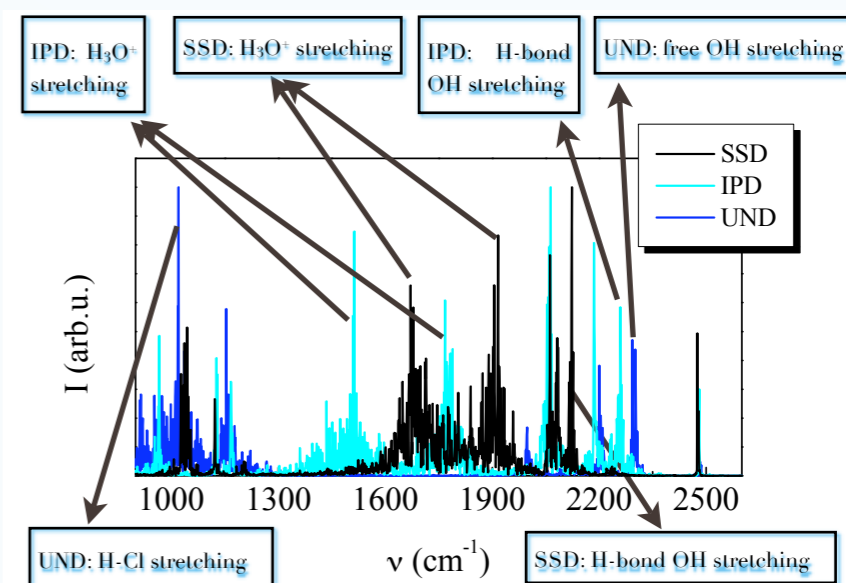
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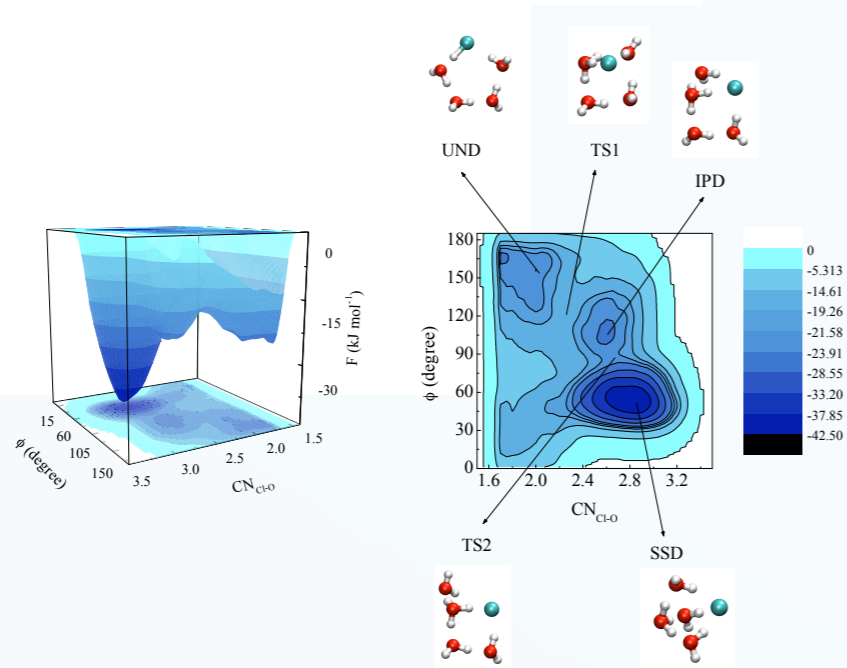


## IR Spectra:

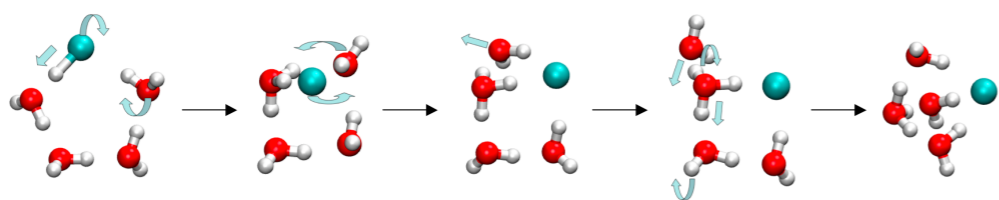


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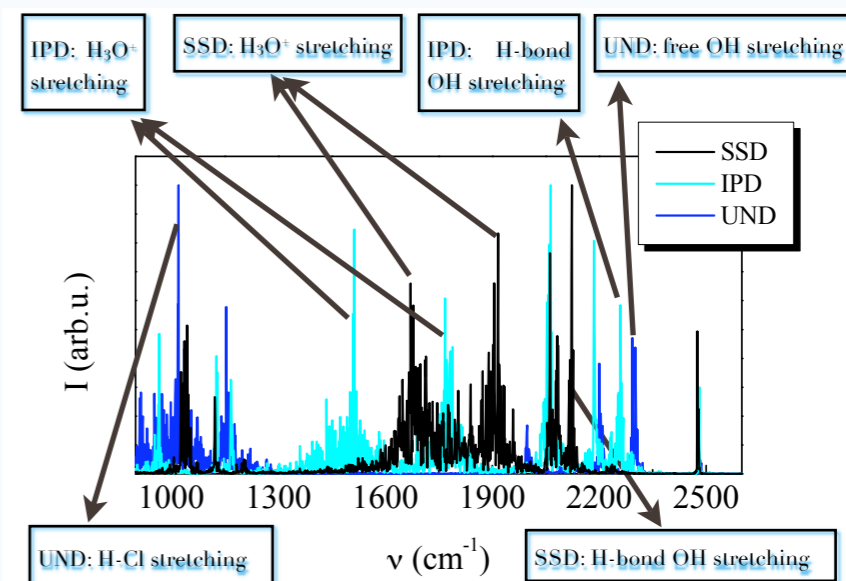
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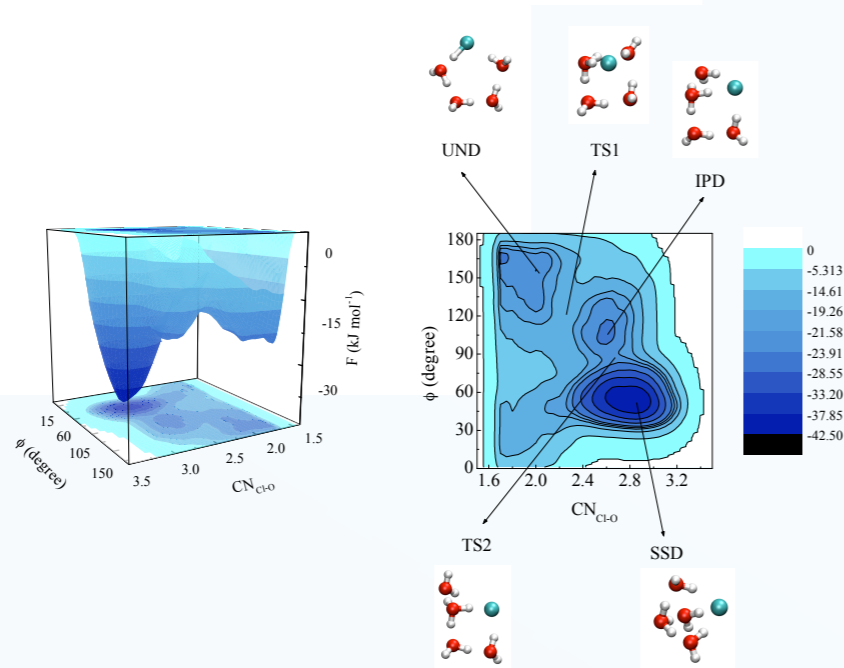


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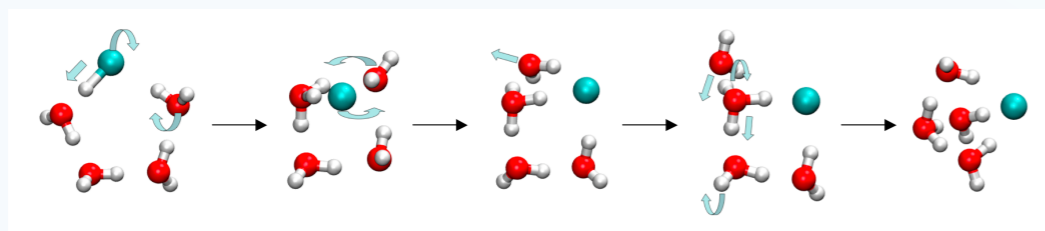
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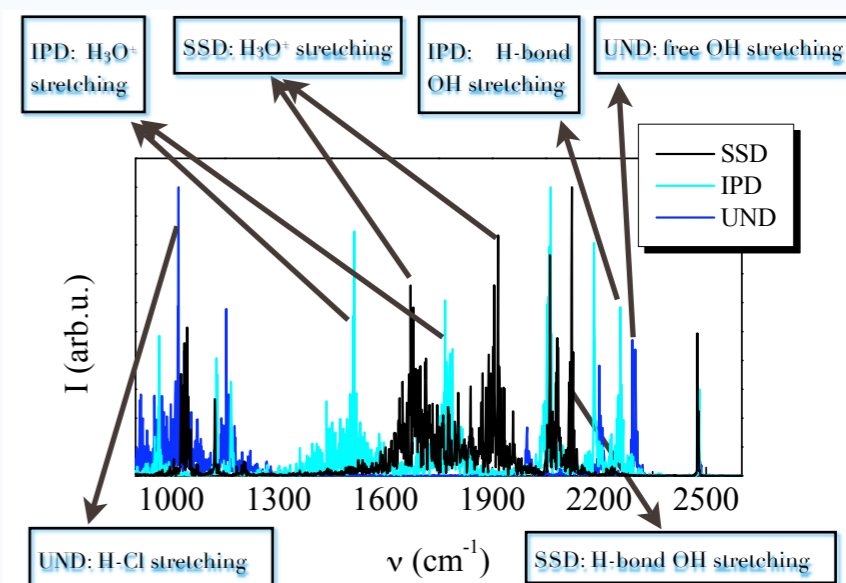
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*Thanks for your attention*