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Hydrogen Bonding: *Ab Initio* Accuracy From Fast Interatomic Gaussian Approximation Potentials

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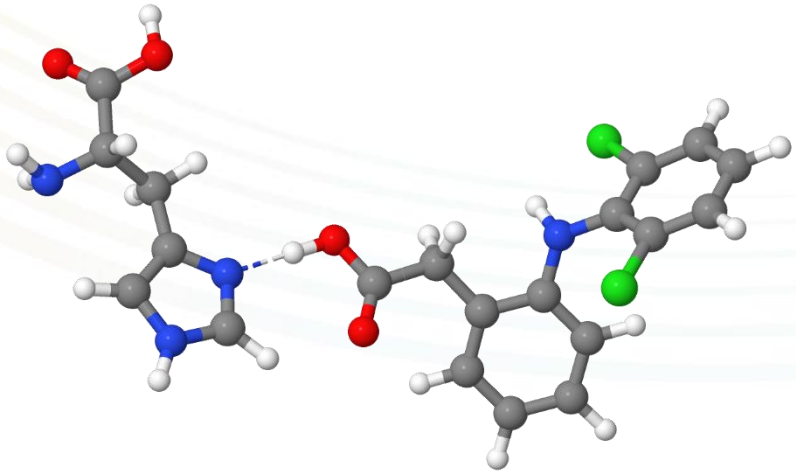
Mario Öeren, PhD – mario@optibrium.com

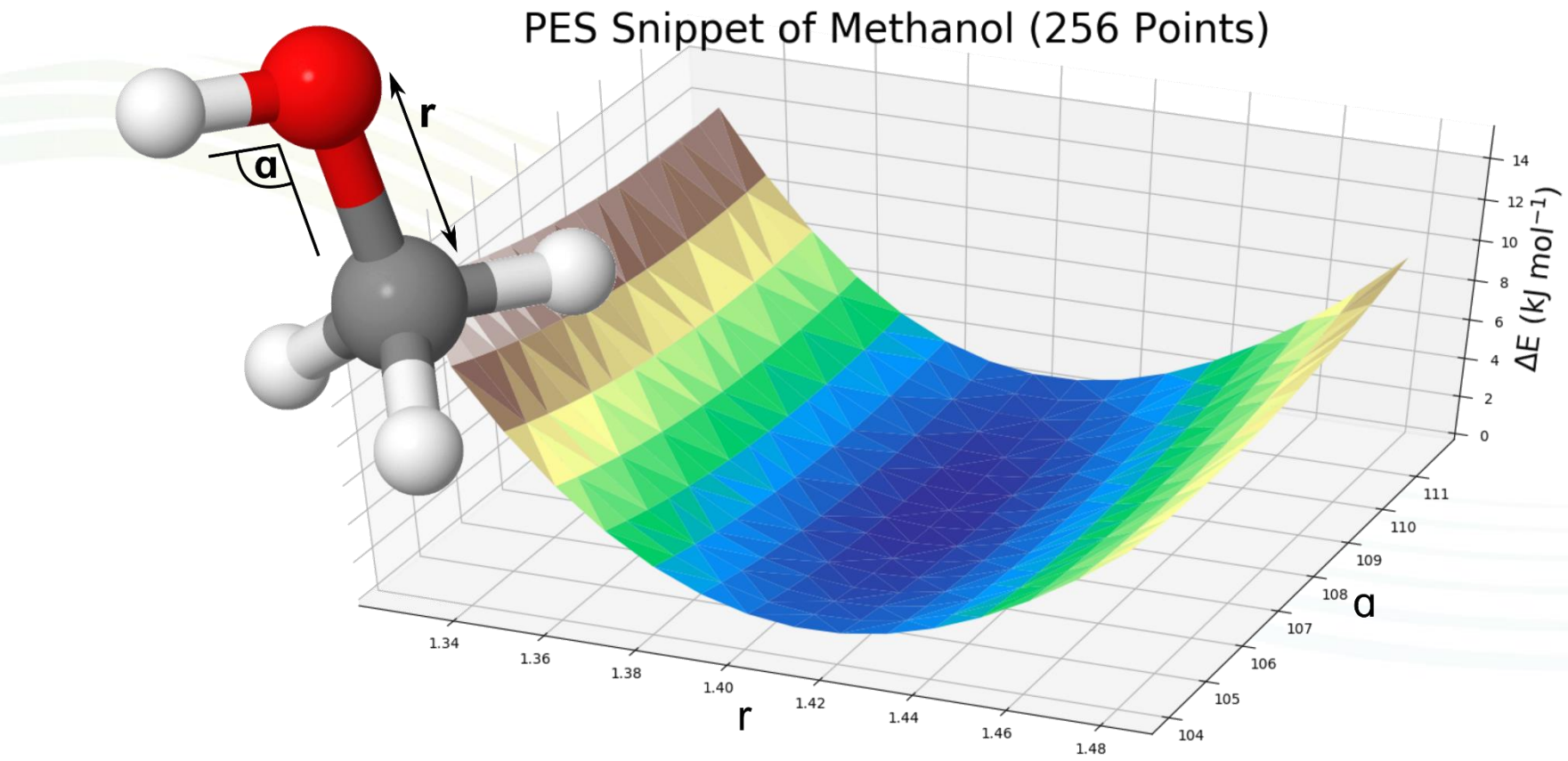
Introduction

- Gaussian Approximation Potential (GAP)
  - A short introduction
  - Practical example
  - *Ab initio* accuracy without electrons
- The Hydrogen Bond Model
  - How GAPs are applied
- Results
  - Accuracy of the model
  - Speed-up
  - Improvements for the model



Gaussian Approximation Potential

B3LYP/def2-SVP



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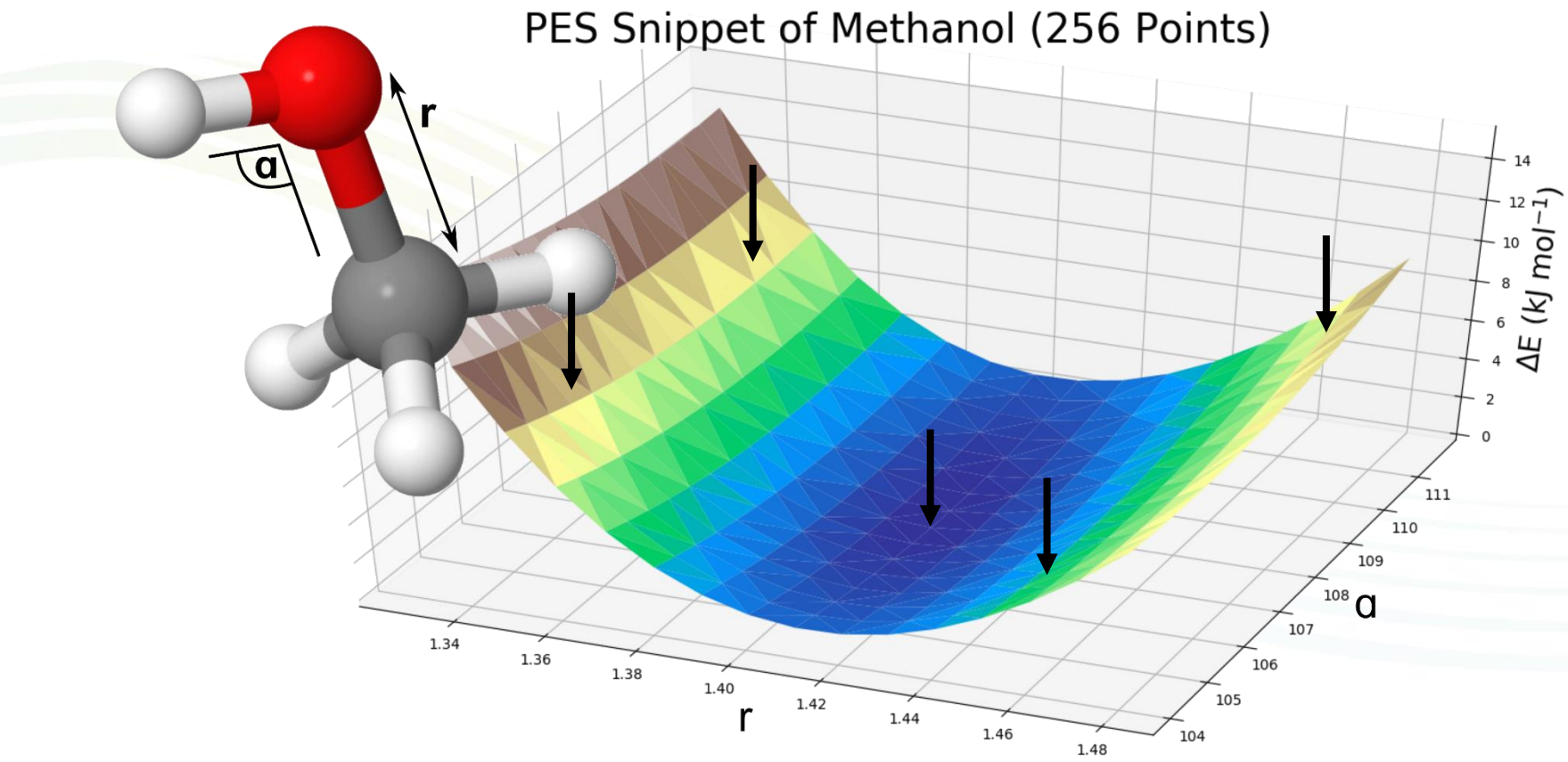
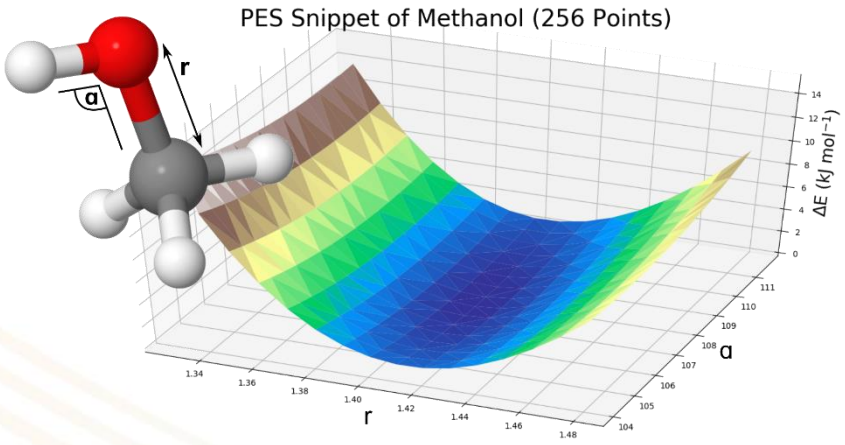
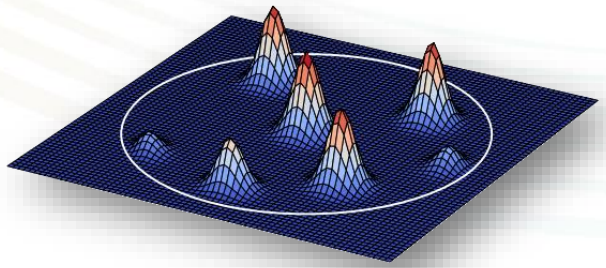


Gaussian Approximation Potential

- Input from an *ab-initio* calculation:
  - Cartesian Coordinates
  - Energy Values
  - Force Values
- Representation of geometry
  - Invariant with respect to permutational, rotational, reflectional and translational symmetry
- Smooth Overlap of Atomic Positions (SOAP)
  - Finite cut-off
  - Complicated environments
  - Size of the system does not matter
- Interatomic potential fit using Gaussian Processes
  - Gaussian Approximation Potential (GAP)

B3LYP/def2-SVP





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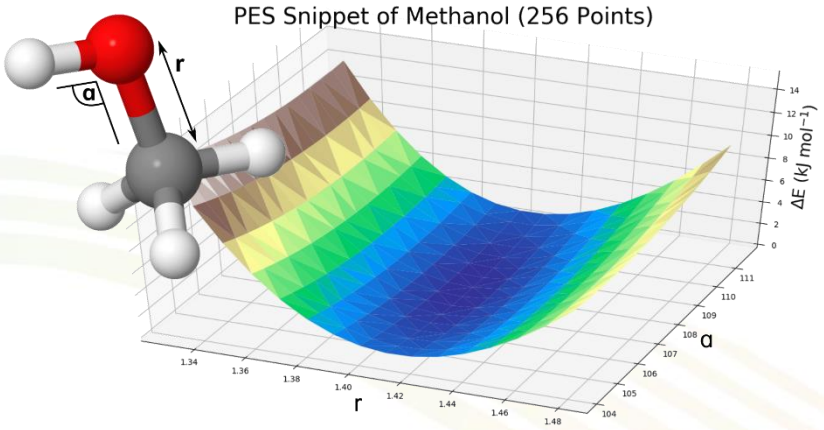
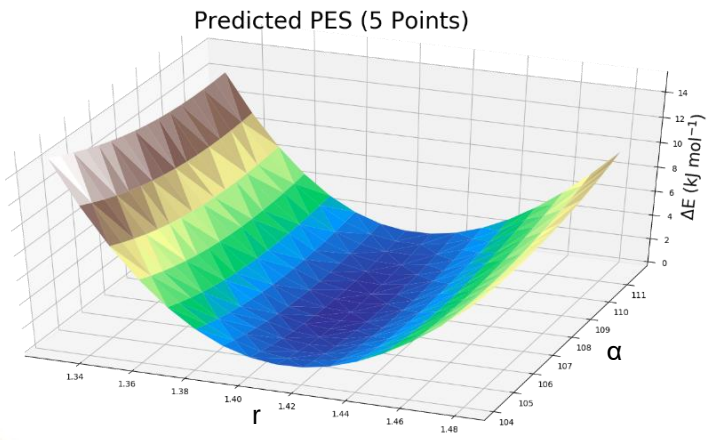
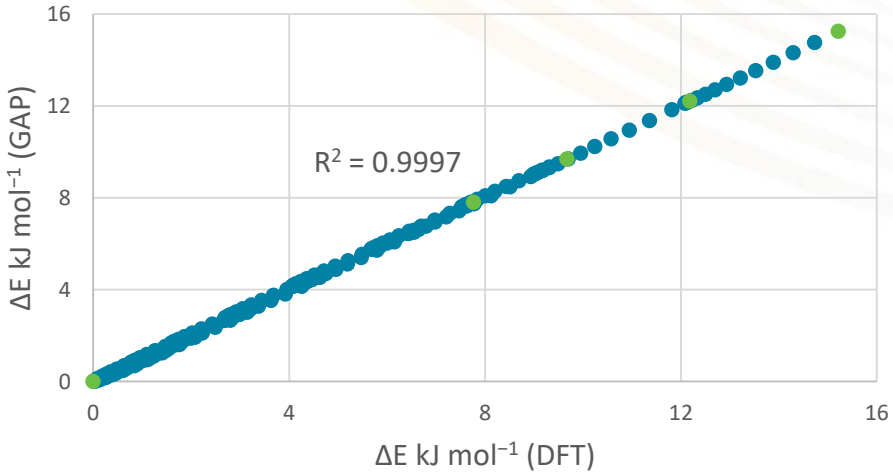




B3LYP/def2-SVP

GAP (Energy, Forces)



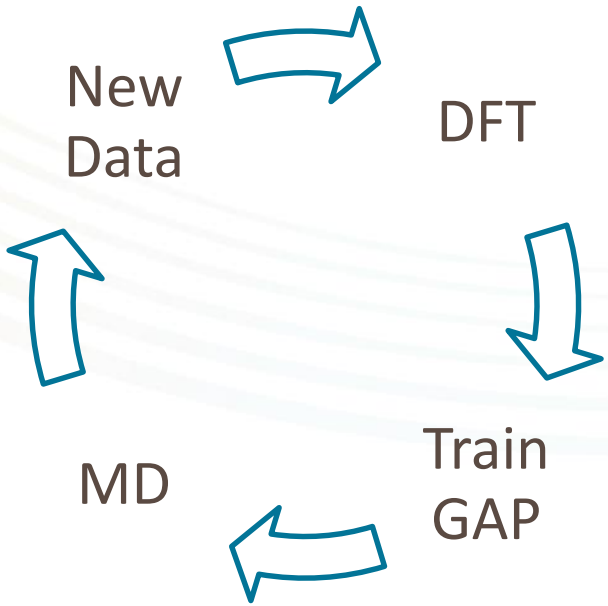
- Test Set (251 Points)
- Training Set (5 Points)

ΔE is the relative energy value (compared to the conformation with the lowest energy value)

GAP for Methanol

12 Degrees of Freedom!

- How to explore the PES (obtain data points)
  - Molecular dynamics simulation
  - Single point calculations of MD snapshots

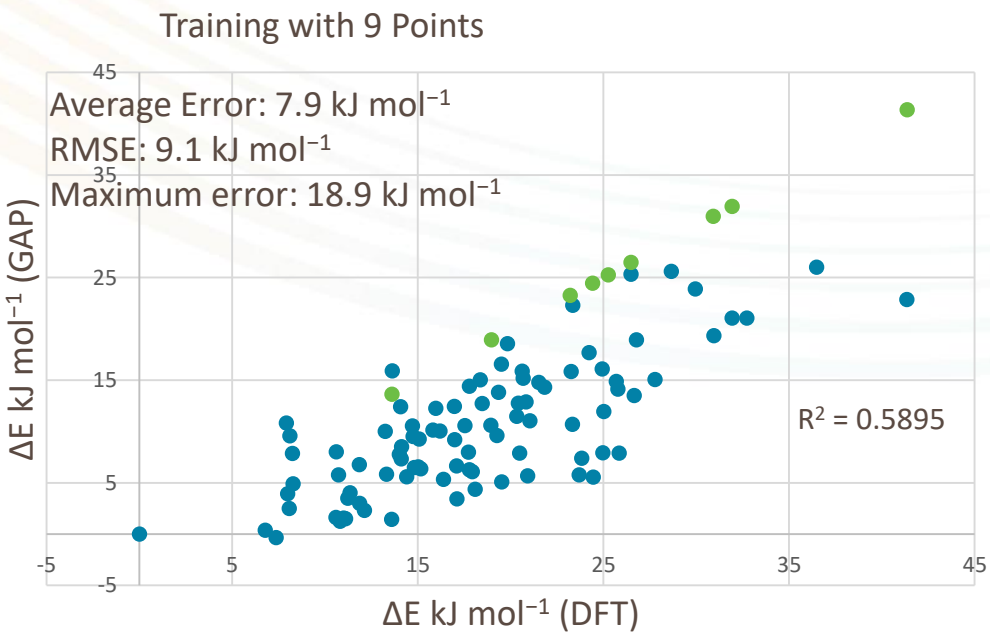


ΔE is the relative energy value

GAP for Methanol

12 Degrees of Freedom!

- How to explore the PES (obtain data points)
  - Molecular dynamics simulation
  - Single point calculations of MD snapshots
- Training and testing
  - 100 initial points
  - 1000 points for testing



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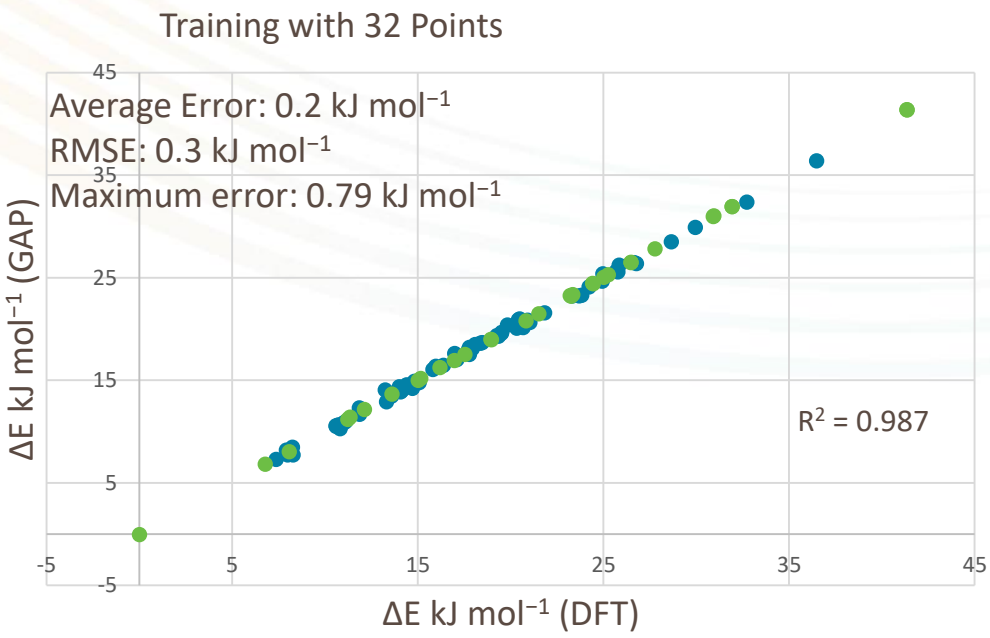

ΔE is the relative energy value

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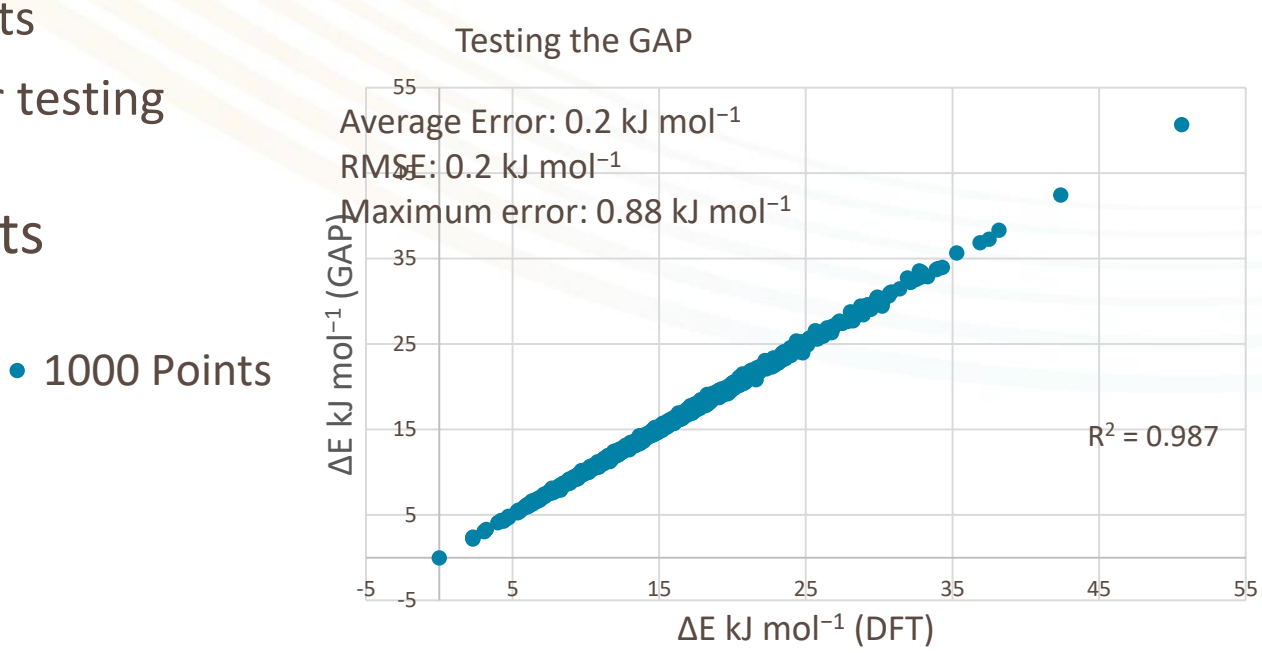
12 Degrees of Freedom!

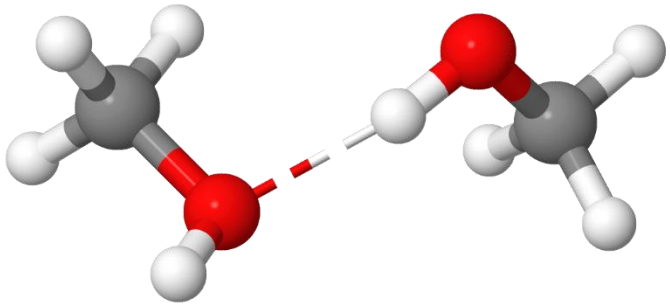
- How to explore the PES (obtain data points)
  - Molecular dynamics simulation
  - Single point calculations of MD snapshots
- Training and testing
  - 100 initial points
  - 1000 points for testing
- 46 training points



ΔE is the relative energy value

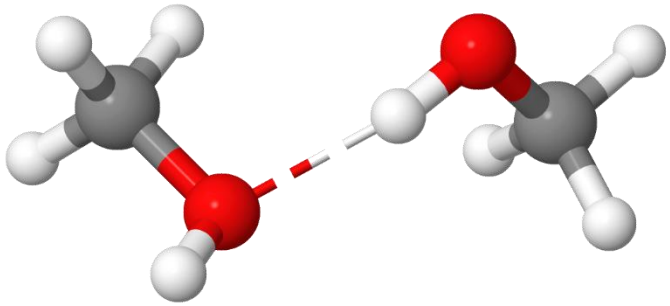
Methanol Dimer

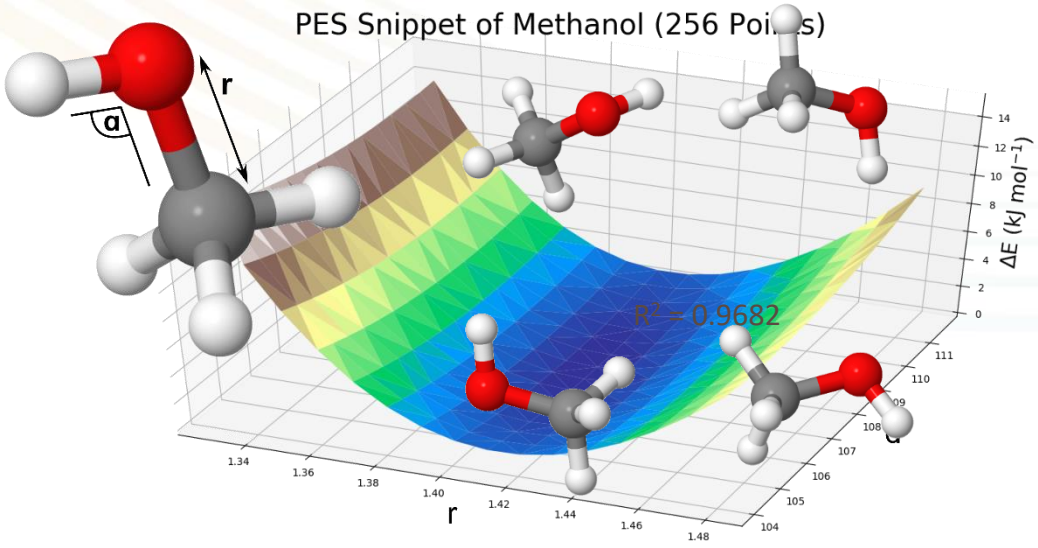
- Complicated PES
  - 25 degrees of freedom
  - Hydrogen bond
  - Wide range of conformations



Methanol Dimer

- Complicated PES
  - 25 degrees of freedom
  - Hydrogen bond
  - Wide range of conformations
    - 3.5×10^{92}
    - 2.4×10^{5}





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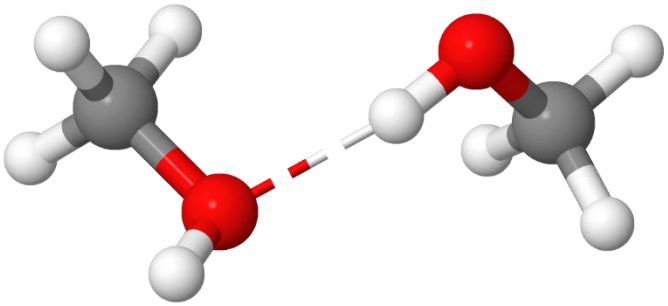
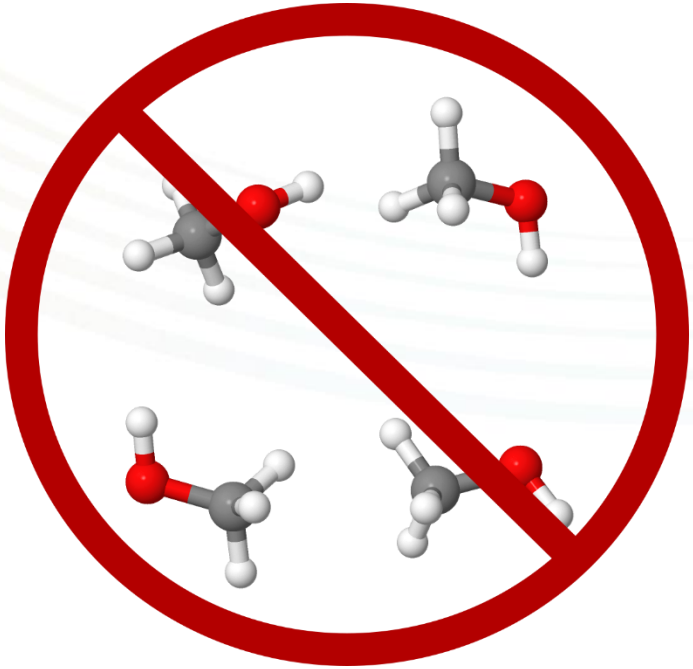


- Simplifications



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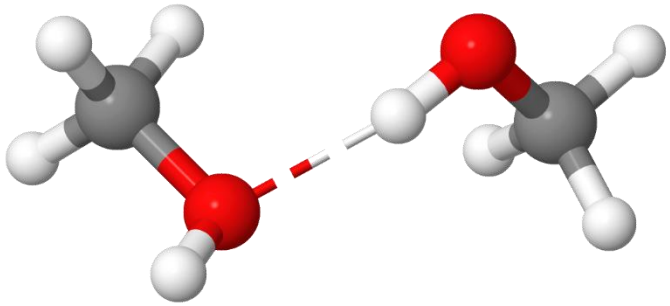
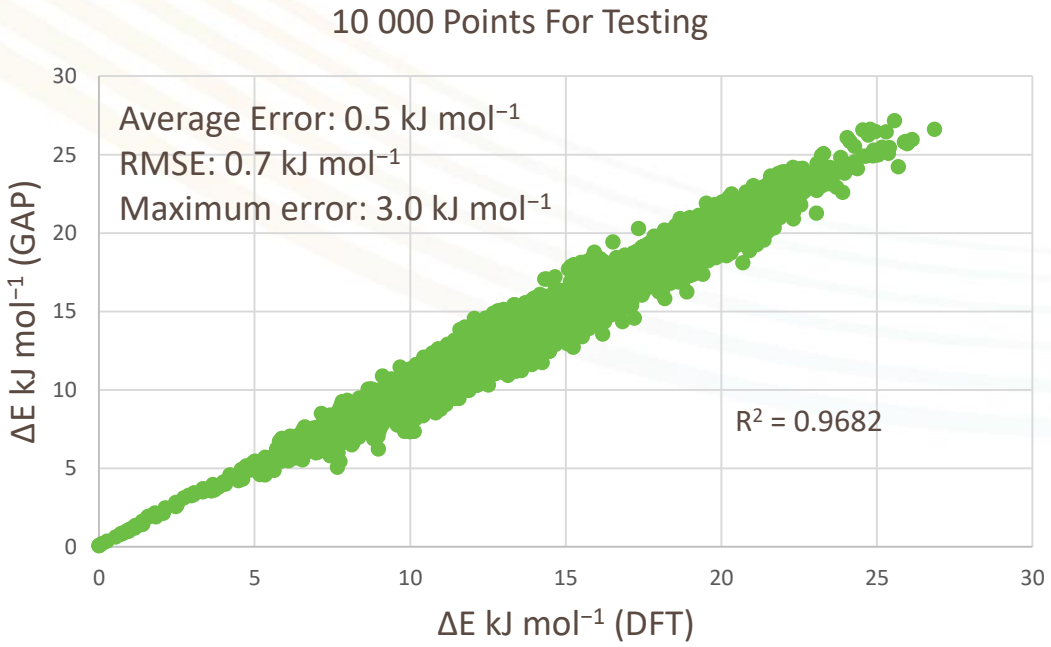
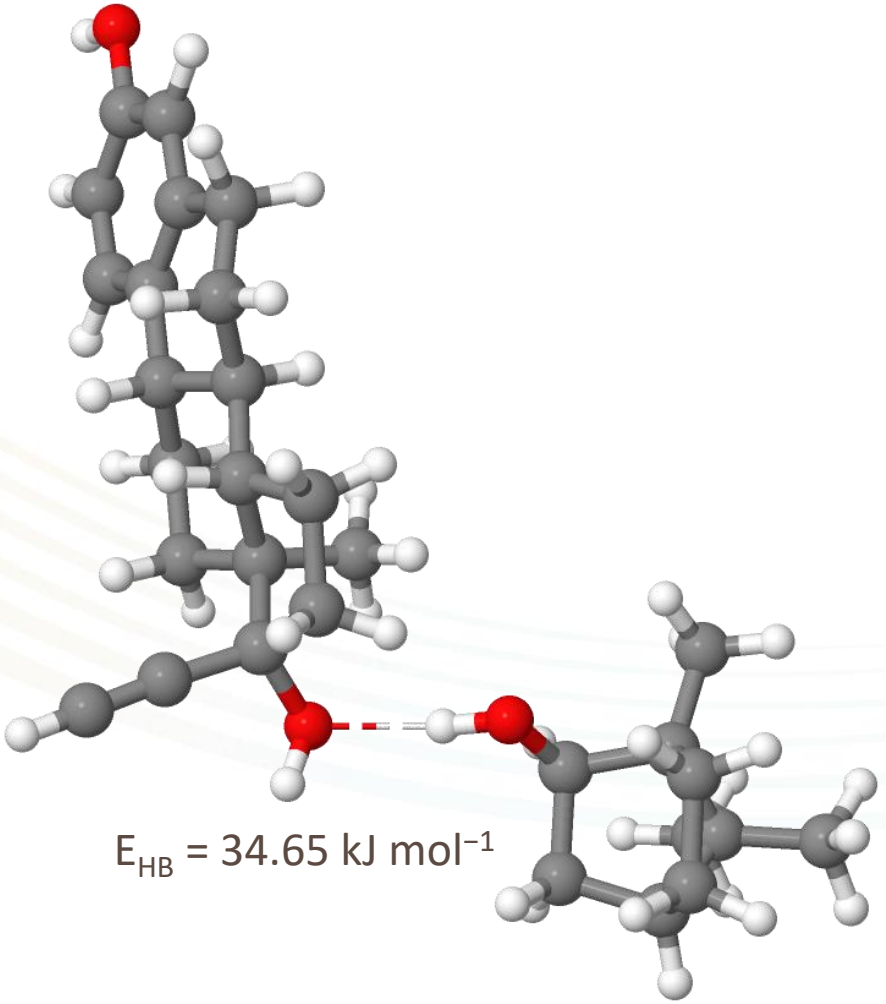


- 1500 Training Points



ΔE is the relative energy value

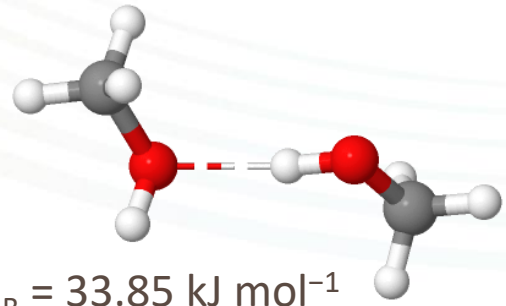
Interaction Potential



E_{HB} = 34.65 kJ mol^{-1}

Interaction Potential

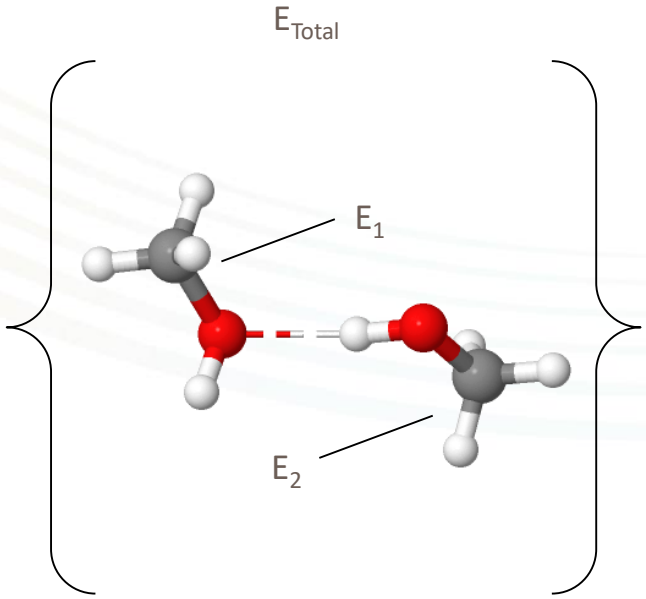
- Form a fragment based system



E_{HB} = 33.85 kJ mol^{-1}

Interaction Potential

- Form a fragment based system
- Hydrogen bond energy
  - Methanol molecules
  - Methanol dimer



$$E_{HB} = E_{Total} - E_1 - E_2$$

Interaction Potential

- Form a fragment based system
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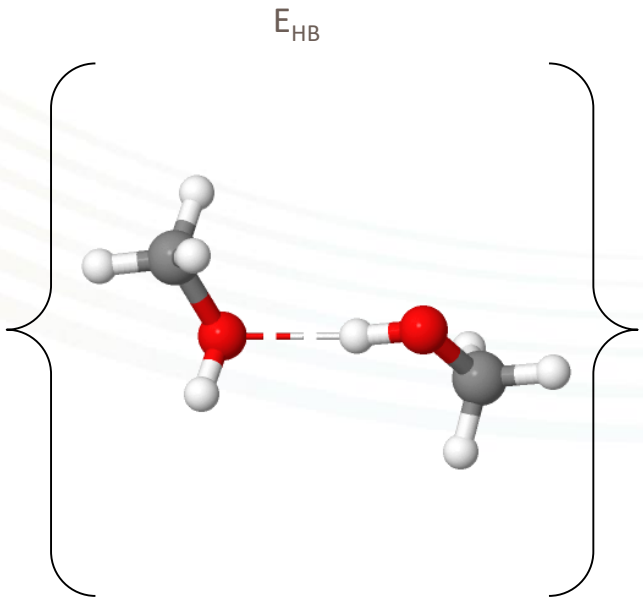
- Interaction potential
  - Train potential with E_{HB}
- Advantages
  - More accurate
  - Reduced time



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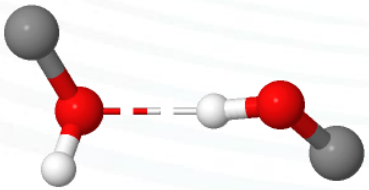

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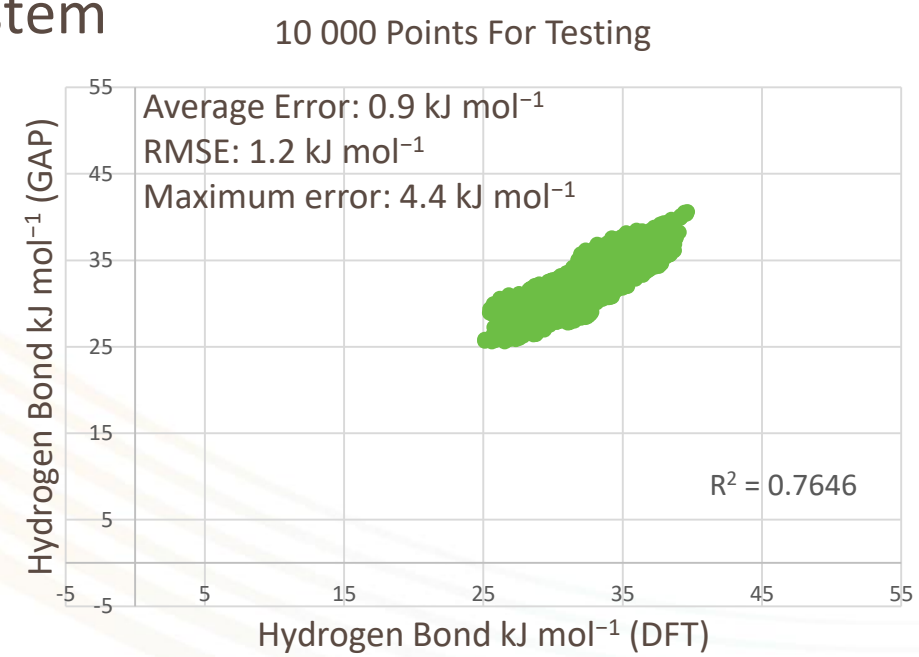

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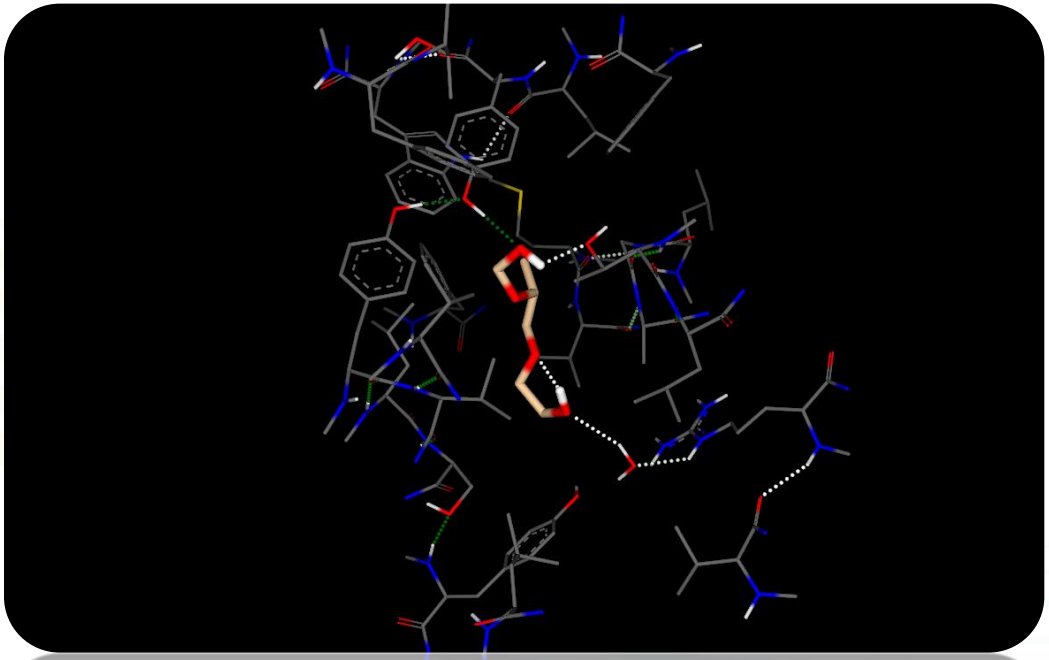

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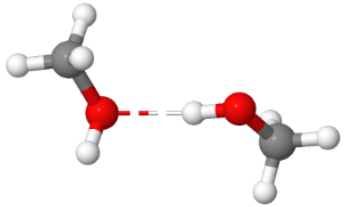
Summary

- Hydrogen bonding model – a*b initio* accuracy using GAPs
  - Error (RMSE): 1.2 kJ mol^{-1}
  - Time gain: 120 seconds (DFT), 0.02 seconds (GAP)



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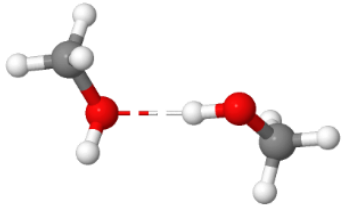
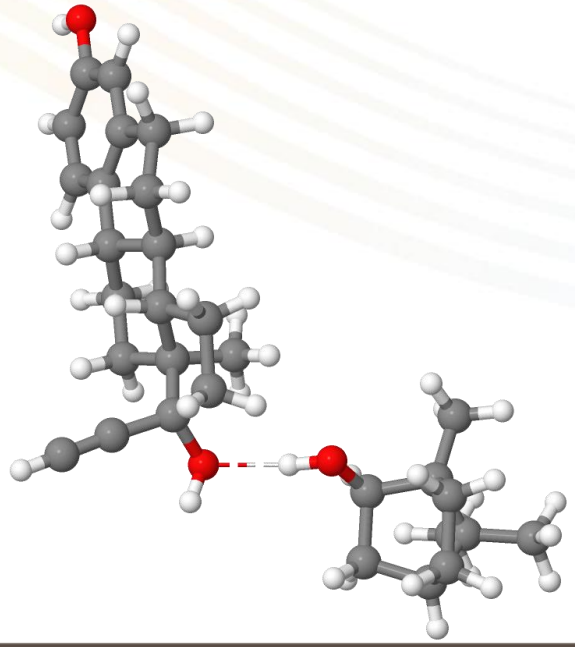


  - Big molecules (12)

    Average Error: 0.54 kJ mol^{-1}, RMSE: 0.66 kJ mol^{-1}, Maximum Error: 1.28 kJ mol^{-1}



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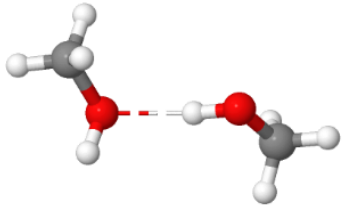

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- Applicability
  - Other dimers

    E.g.

    methanol : formaldehyde
    methanol : formic acid anion
    methanol : primary amine
    methanol : formic acid,
    formic acid : formic acid,
    primary amine : primary amine

  - GAPs have a wide range of applications
  - Any level of theory can be used with GAPs

Future Work

- Über potential
  - Additional dimers found in and between drug molecules and proteins
  - More charged species
  - Combine atom types
  - Reduce the amount of dimers
- Additional interactions
  - Complex dimers
  - Third monomer
- Predict errors of the model

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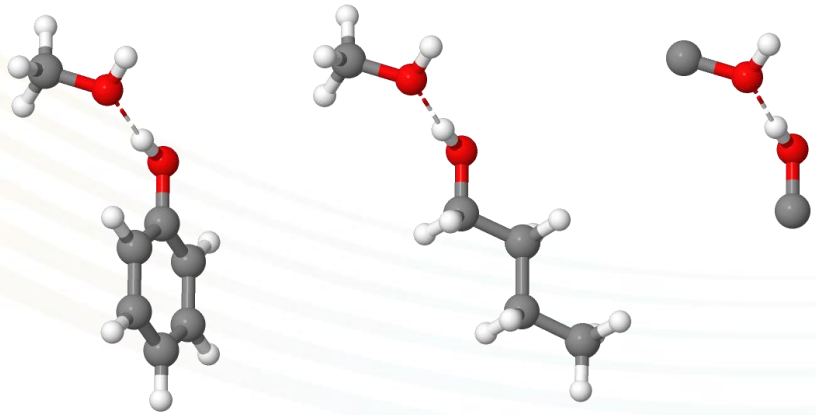

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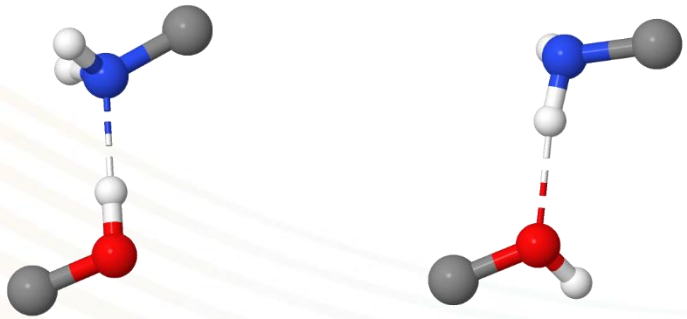

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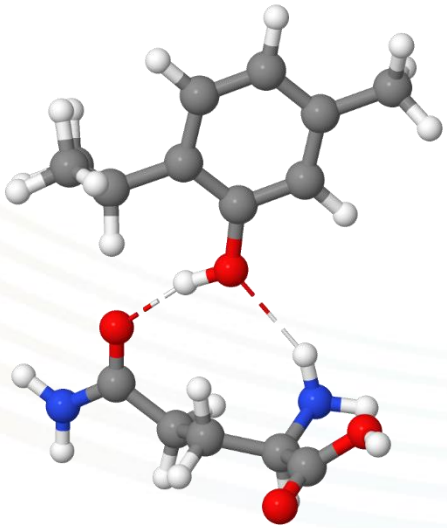

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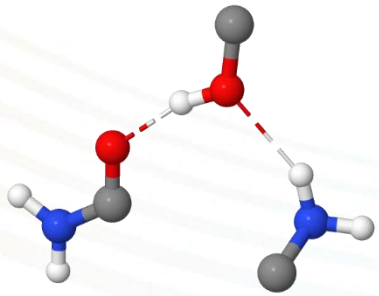

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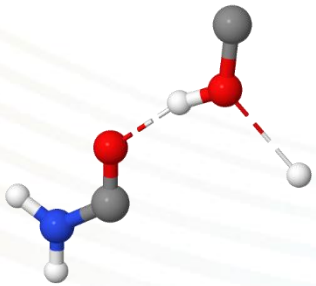

Thank You

- Peter Hunt
- Gábor Csányi
- David Ponting
- Matthew Segall

GAP
SOAP

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