NEFARIOUS SSH ACCESS

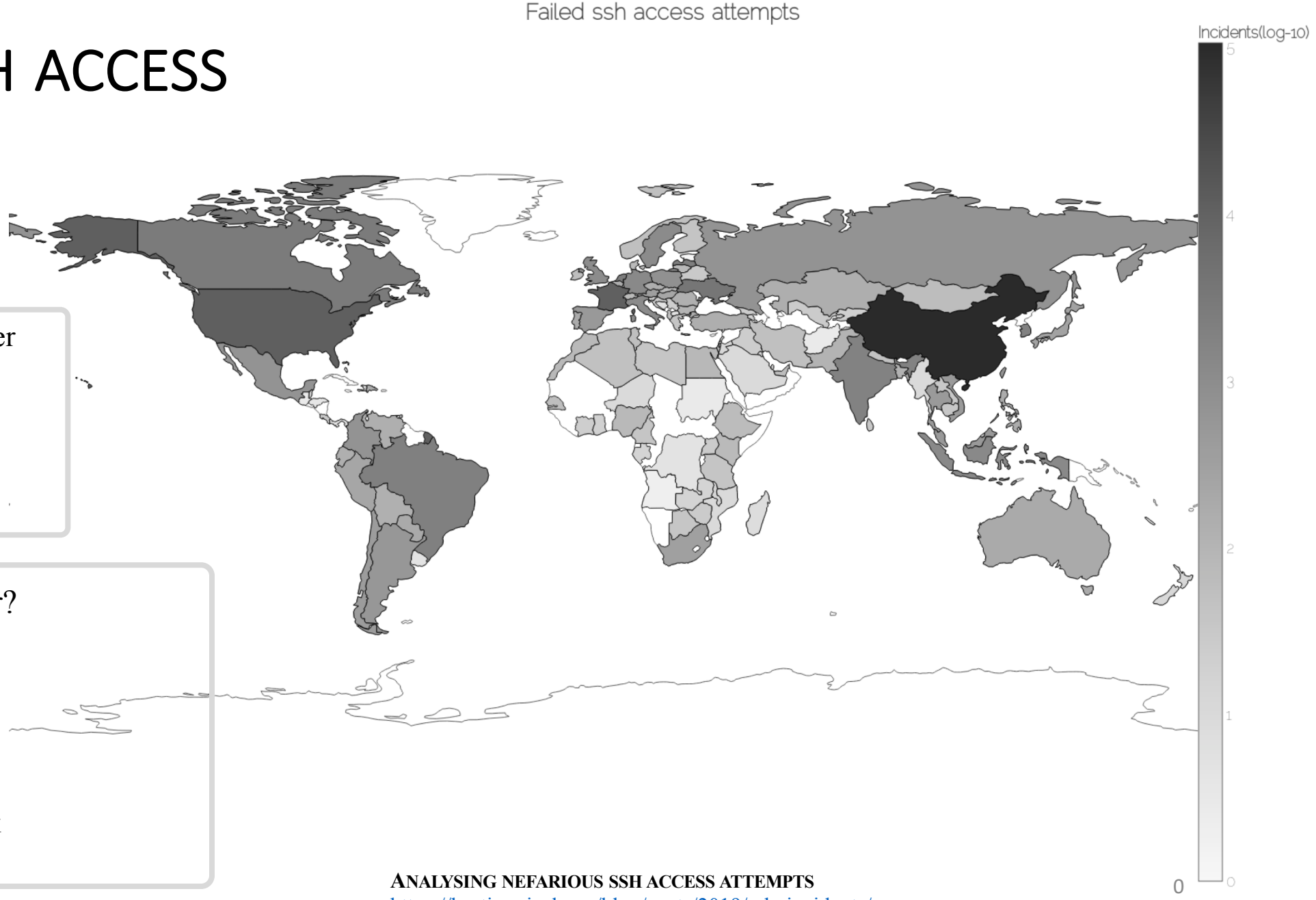
For a single server with public IP, within one month, among 983,892 ssh attempt, 167,911 are considered as nefarious ssh connection attempt.

Valid User	Invalid User
1.root (98.42%)	1.admin
2.backup (0.29%)	2.test
3.www-data (0.14%)	3.user
4.ghost (0.11%)	4.ubuntu
5.nobody (0.08%)	

How to protect your server?

```
vi /etc/ssh/sshd_config
```

1. Disable root login
2. PasswordAuthentication NO
3. Hide server into UF network



ANALYSING NEFARIOUS SSH ACCESS ATTEMPTS
https://bastian.rieck.me/blog/posts/2019/ssh_incidents/

Predicting Molecular Orbital Energies with Deep Learning

Jinze (Richard) Xue

2020.01.21

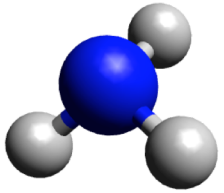
UF | Roitberg Group
Computational Chemistry

Overview

1. Introduction
2. Problem Analysis
3. Model
4. Dataset
5. Result
6. Future Work

Introduction: ANI

Standard QM



NH_3

0 1			
H	5.28092	4.45771	5.58748
H	3.95200	3.80817	6.26654
H	3.95199	4.19440	4.68543
N	4.26359	4.51440	5.60133

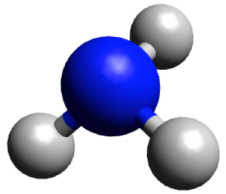
Gaussian / ORCA / PSI4

With given basis set and
level of theory (HF / DFT / CCSD)

seconds / minutes / days

Total Energy

ANI



NH_3

0 1			
H	5.28092	4.45771	5.58748
H	3.95200	3.80817	6.26654
H	3.95199	4.19440	4.68543
N	4.26359	4.51440	5.60133

Millions of conformations
Thousands of molecules

A huge non-linear function
with 326,660 parameters

ANI
Neural Network

Trained to a given basis set and
level of theory (HF / DFT / CCSD)

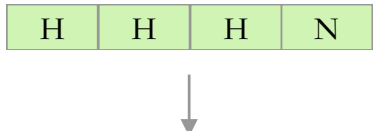
Total Energy

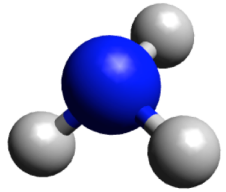
With RMSE about 2 kcal/mol

RMSE: Root Mean Squared Error

Current ANI Model

Input: coordinates and species



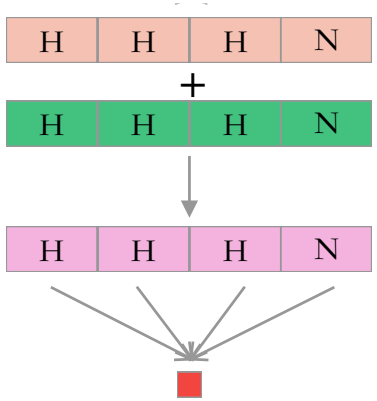


NH_3

Coordinates and species
coordinates size: 3 (x, y, z)
species size: 1

ANI
Neural Network

Atom Energy Correction by ANI
+
Atom base Energy



[0.0362, 0.0339, 0.0012, -0.1014]

[-0.6009, -0.6009, -0.6009, -54.7077]

[-0.5964, -0.5967, -0.6008, -54.7204]

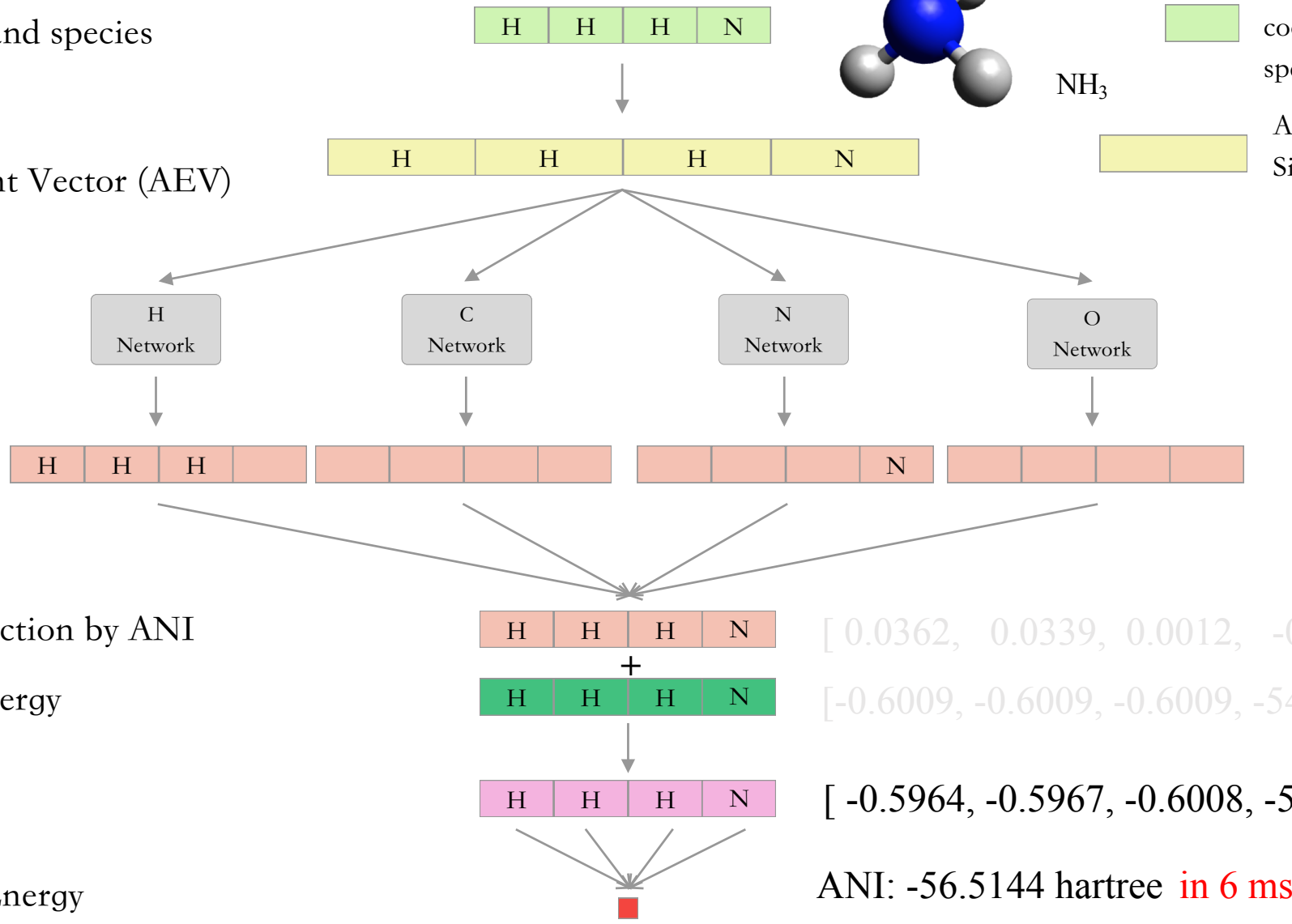
Output: Molecule Energy

ANI: -56.5144 hartree

Molecule Energy
Size: 1

Current ANI Model

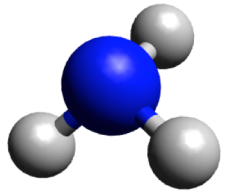
Input: coordinates and species



Introduction: MO (Quantum view)

Atom	1s	2s	$2p_x$	$2p_y$	$2p_z$	d	total
N	1	2	2	2	2	6	15
H	2						2

21



NH_3

6-31G(d) basis set

```
0 1
H       5.28092   4.45771   5.58748
H       3.95200   3.80817   6.26654
H       3.95199   4.19440   4.68543
N       4.26359   4.51440   5.60133
```

H: 2 — ϕ_1 ϕ_2 | H: 2 — ϕ_3 ϕ_4 | H: 2 — ϕ_5 ϕ_6 | N: 15 — ϕ_7 … ϕ_{21}

Solve $\mathbf{H}\boldsymbol{c} = \epsilon\mathbf{S}\boldsymbol{c}$

Eigenvector: Orbital coefficients Eigenvalue: Orbital Energy

$$\psi_m = c_m^1\,\phi_1 + c_m^2\,\phi_2 + c_m^3\,\phi_3 + c_m^4\,\phi_4 + c_m^5\,\phi_5 + c_m^6\,\phi_6 + c_m^7\,\phi_7 + \ldots + c_m^{21}\,\phi_{21} \qquad \epsilon_m$$

5 Occupied Orbitals

$$\psi_1 = c_1^1\,\phi_1 + c_1^2\,\phi_2 + c_1^3\,\phi_3 + c_1^4\,\phi_4 + c_1^5\,\phi_5 + c_1^6\,\phi_6 + c_1^7\,\phi_7 + \ldots + c_1^{21}\,\phi_{21} \qquad \epsilon_1$$

$$\ldots$$

$$\psi_5 = c_5^1\,\phi_1 + c_5^2\,\phi_2 + c_5^3\,\phi_3 + c_5^4\,\phi_4 + c_5^5\,\phi_5 + c_5^6\,\phi_6 + c_5^7\,\phi_7 + \ldots + c_5^{21}\,\phi_{21} \qquad \epsilon_5$$

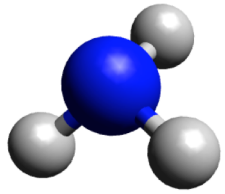
16 Unoccupied (virtual) orbitals

$$\ldots$$

$$\psi_{21} = c_{21}^1\,\phi_1 + c_{21}^2\,\phi_2 + c_{21}^3\,\phi_3 + c_{21}^4\,\phi_4 + c_{21}^5\,\phi_5 + c_{21}^6\,\phi_6 + c_{21}^7\,\phi_7 + \ldots + c_{21}^{21}\,\phi_{21} \qquad \epsilon_{21}$$

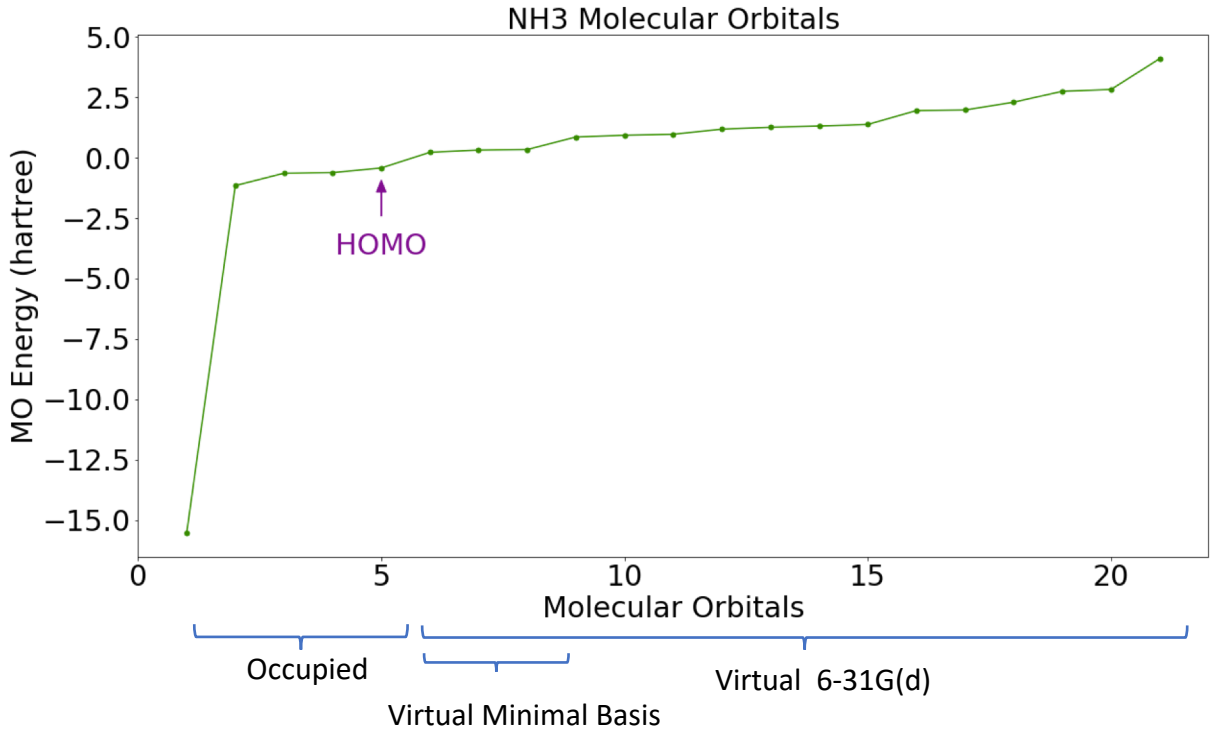
Atom	1s	2s	$2p_x$	$2p_y$	$2p_z$	d	total
N	1	2	2	2	2	6	15
H	2						2

21



NH_3

6-31G(d) basis set



TODO: change font

HF / 6-31g(d)

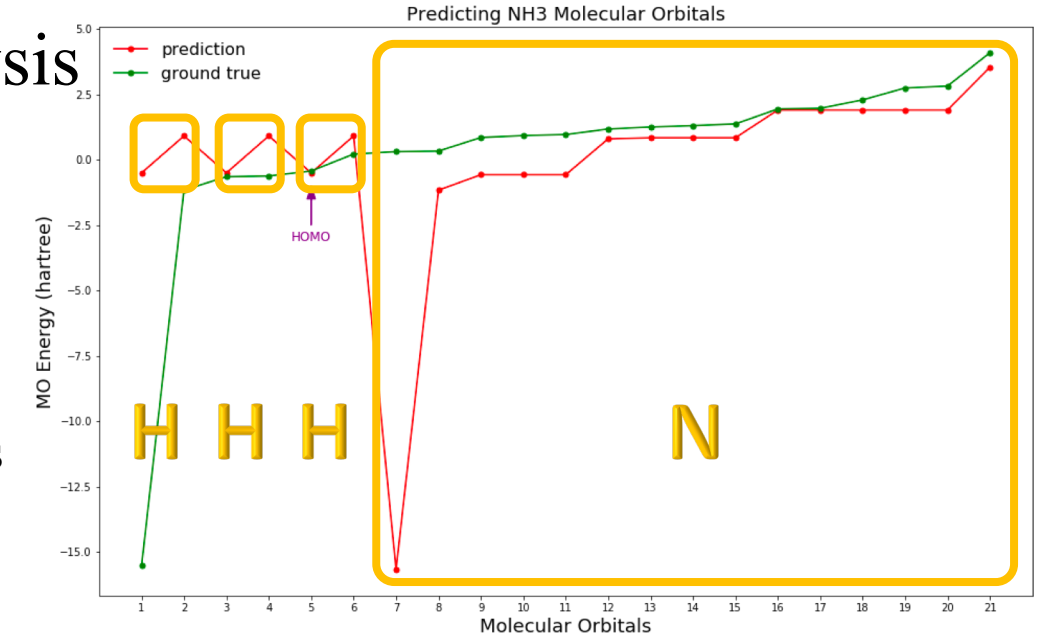
Atom	1s	2s	$2p_x$	$2p_y$	$2p_z$	d	total
N	1	1	1	1	1		5
H	1						1

8

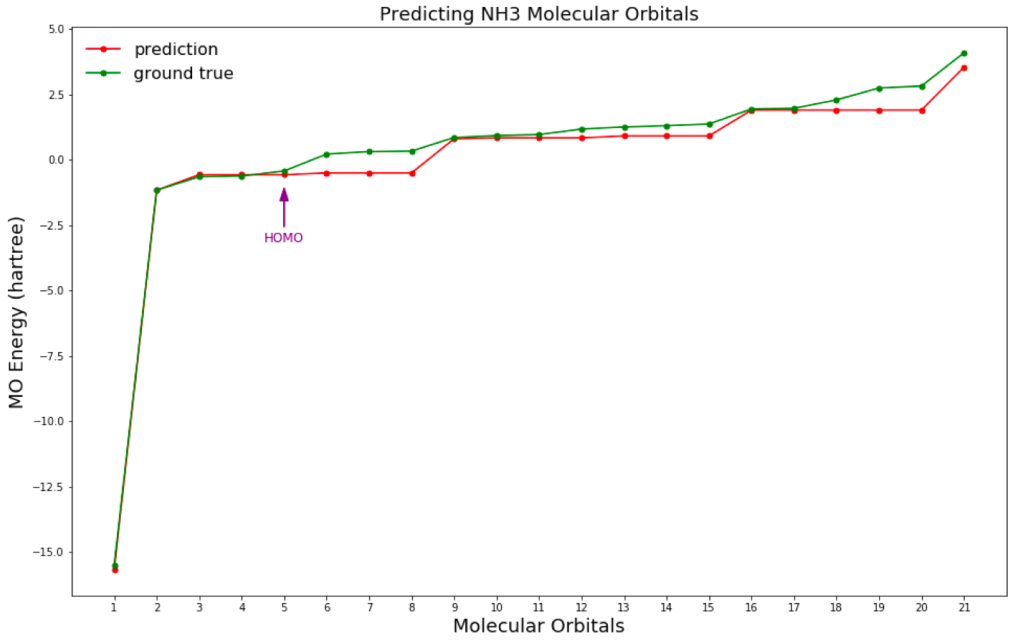
Minimal basis set (STO-3G)

Analysis

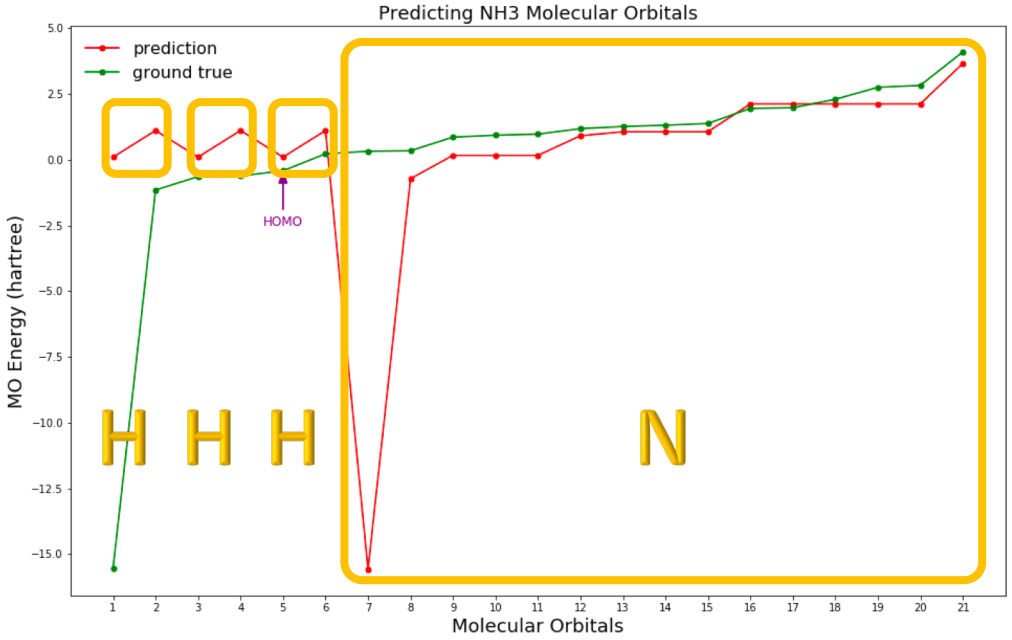
Build from atomic alpha orbitals



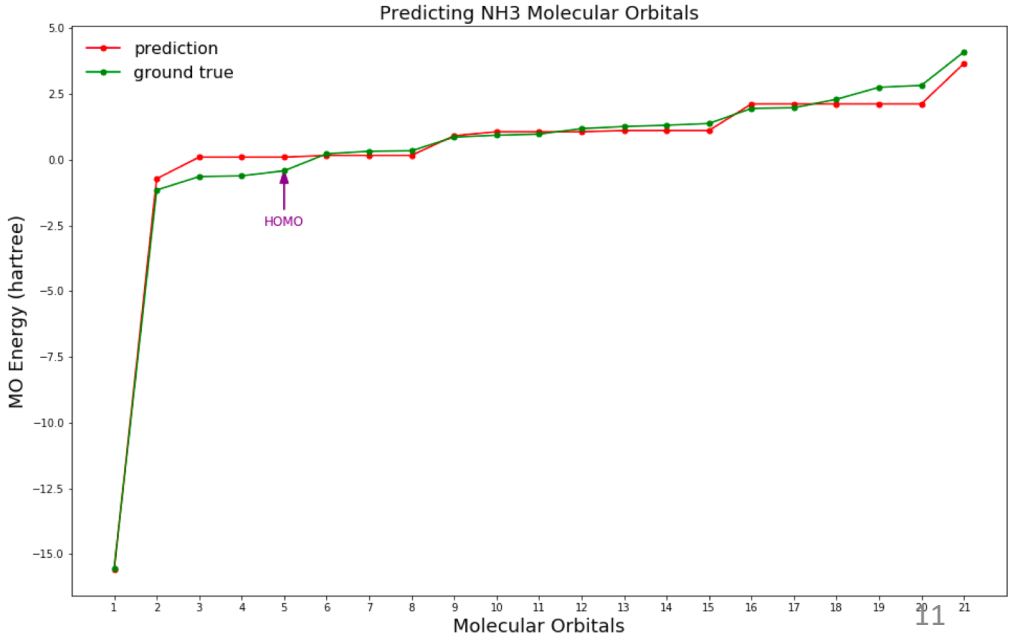
Sort



Build from atomic beta orbitals

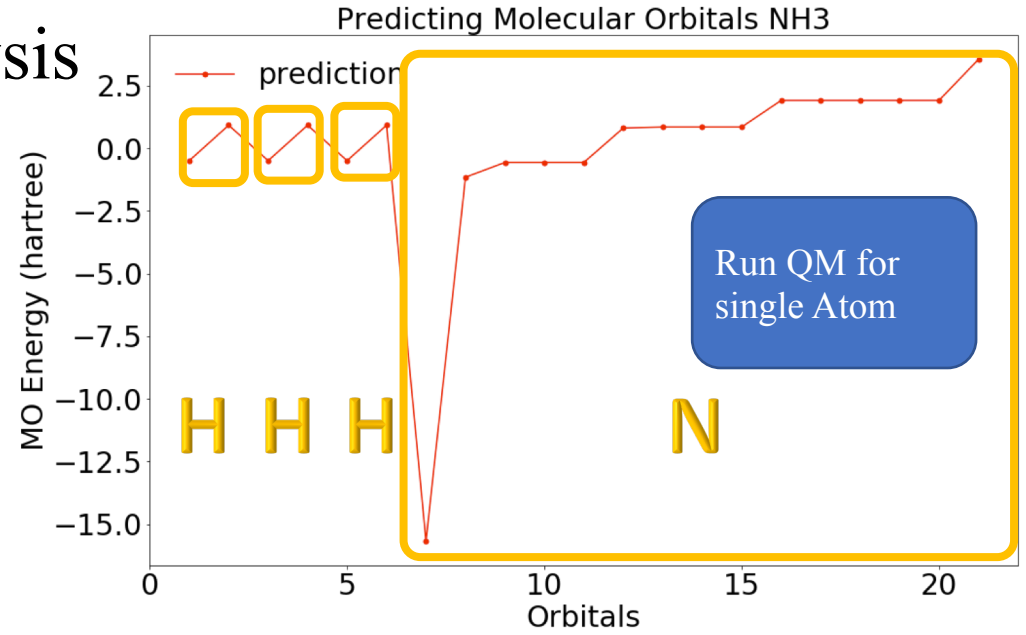


Sort

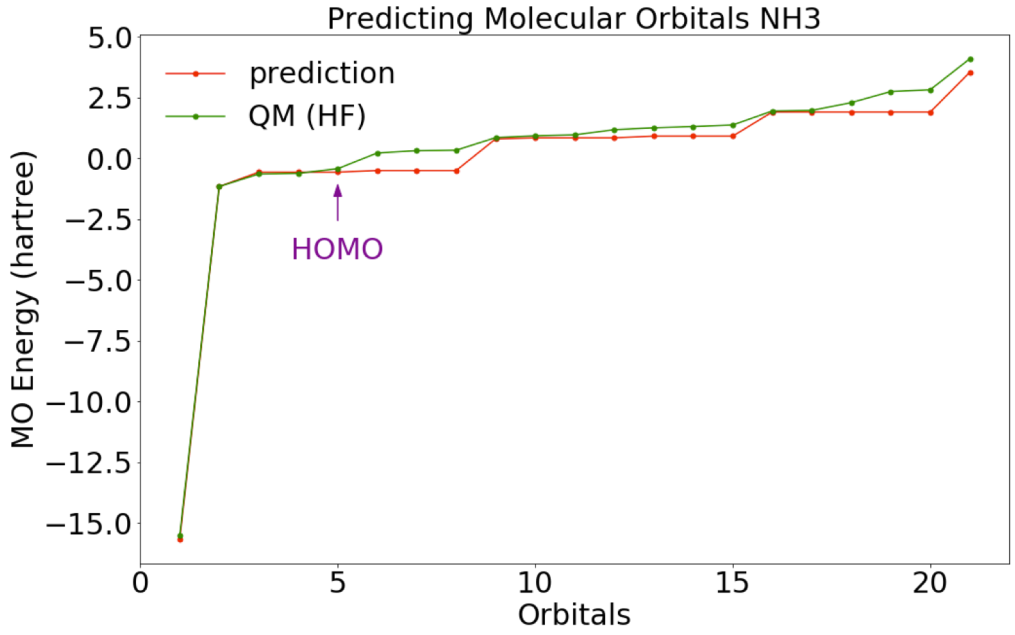


Analysis

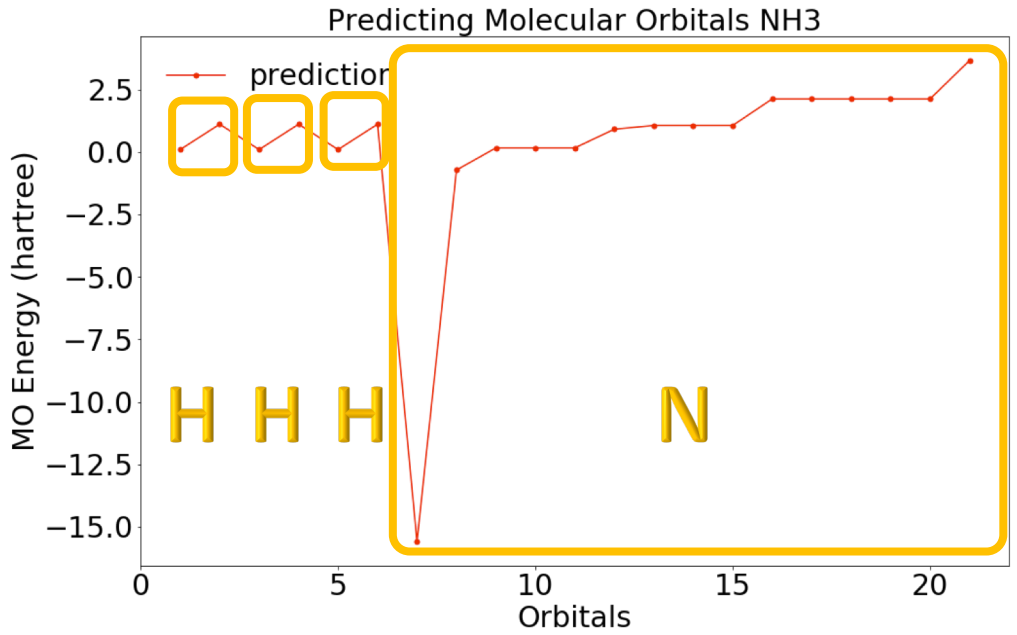
Atomic alpha orbitals



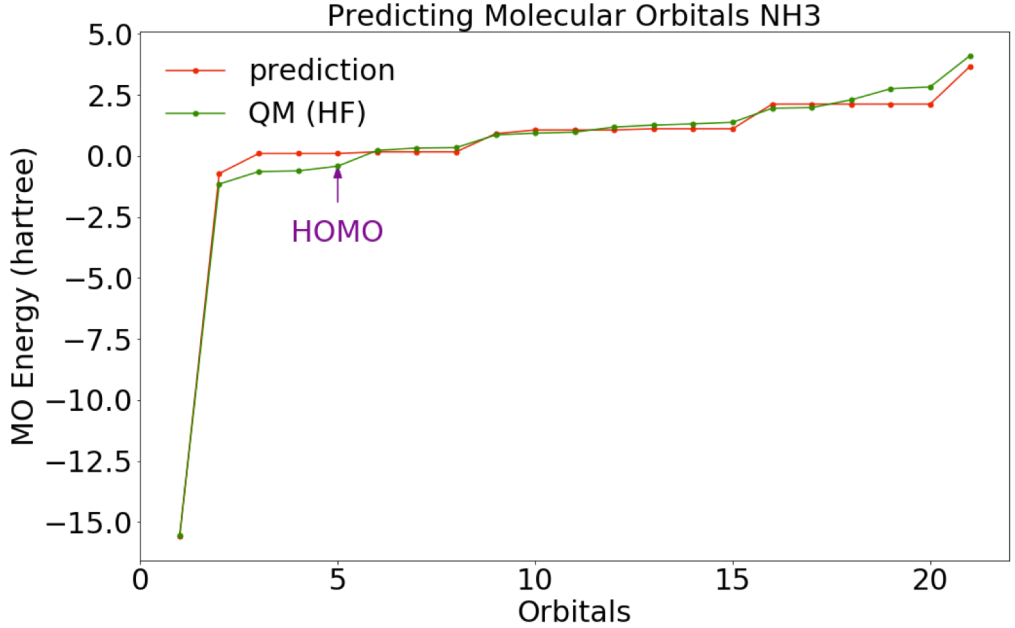
Sort



Atomic beta orbitals

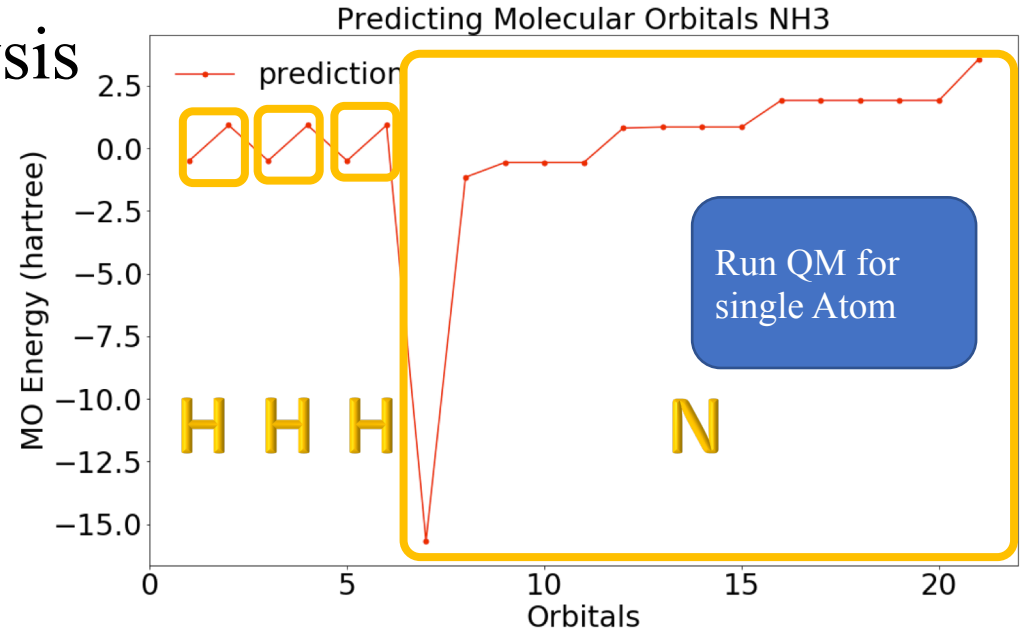


Sort

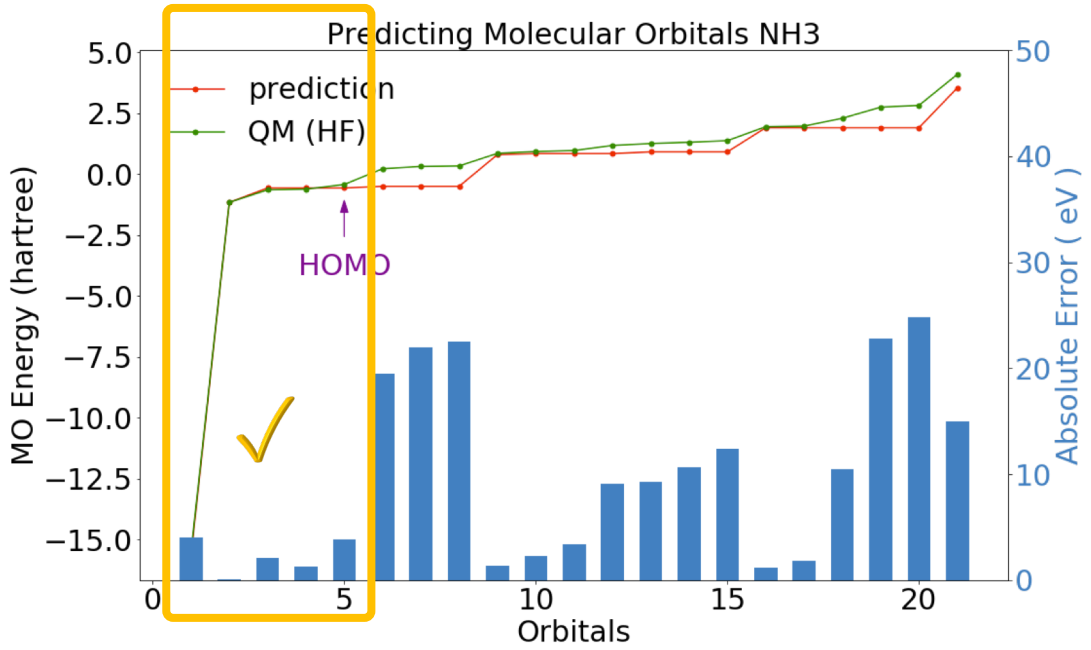


Analysis

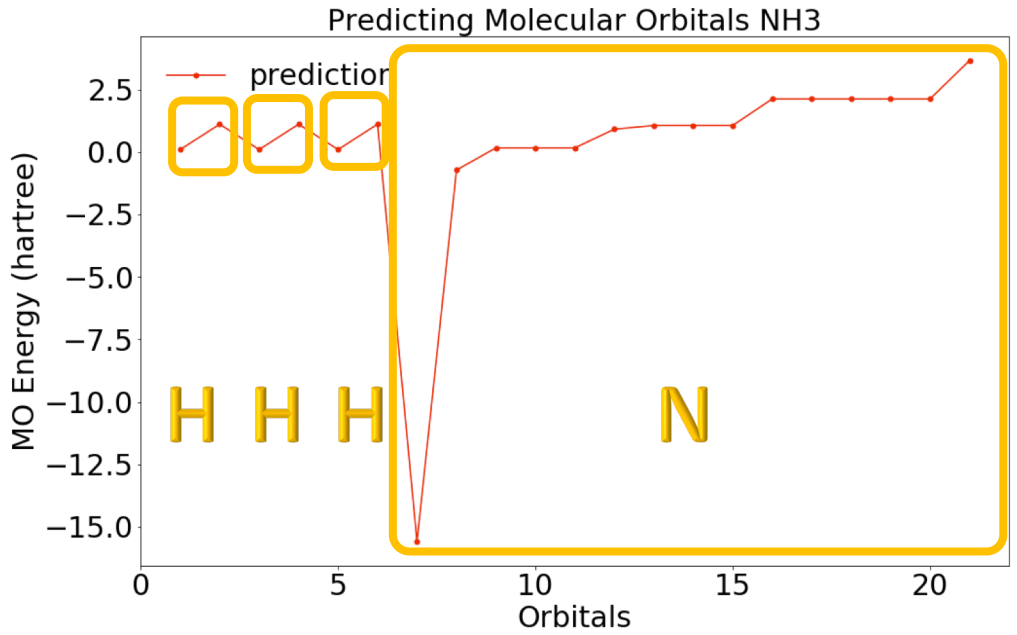
Atomic alpha orbitals



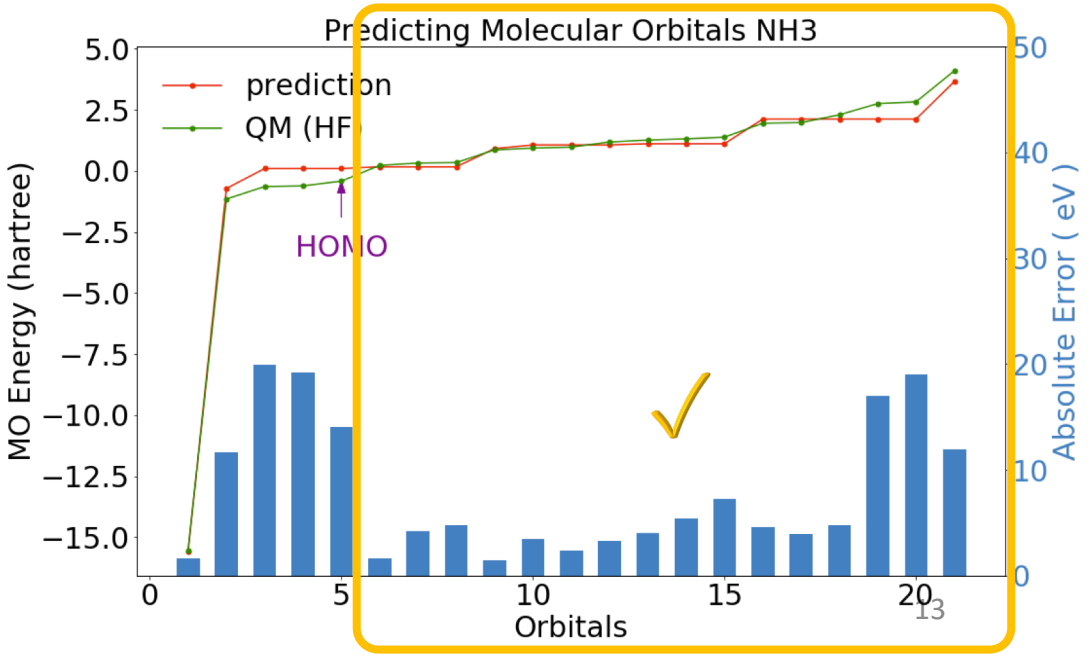
Sort



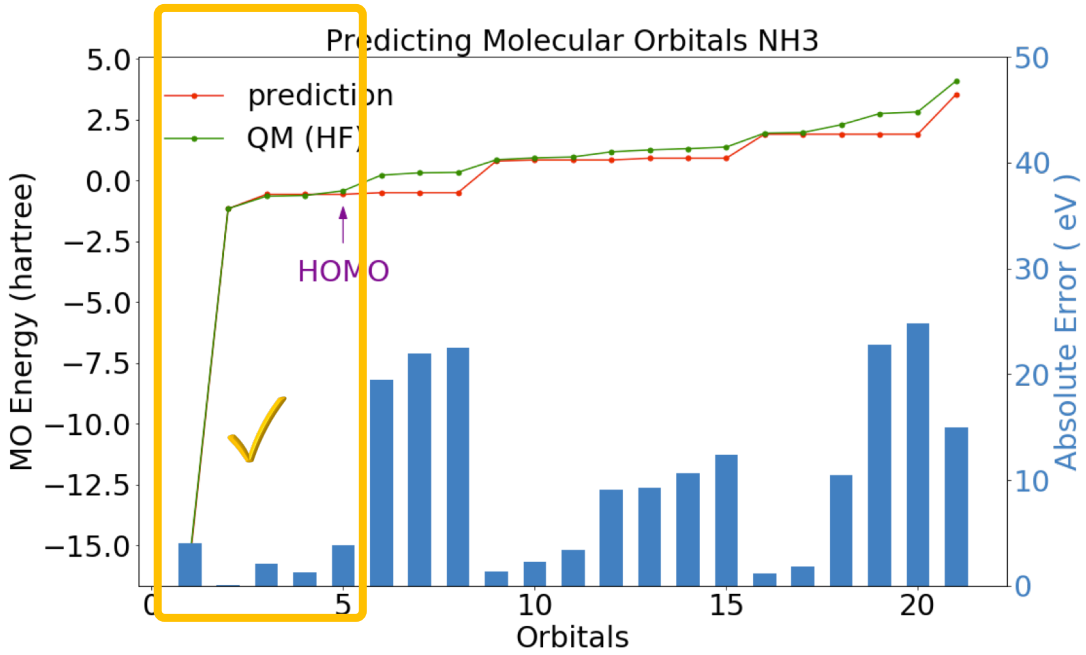
Atomic beta orbitals



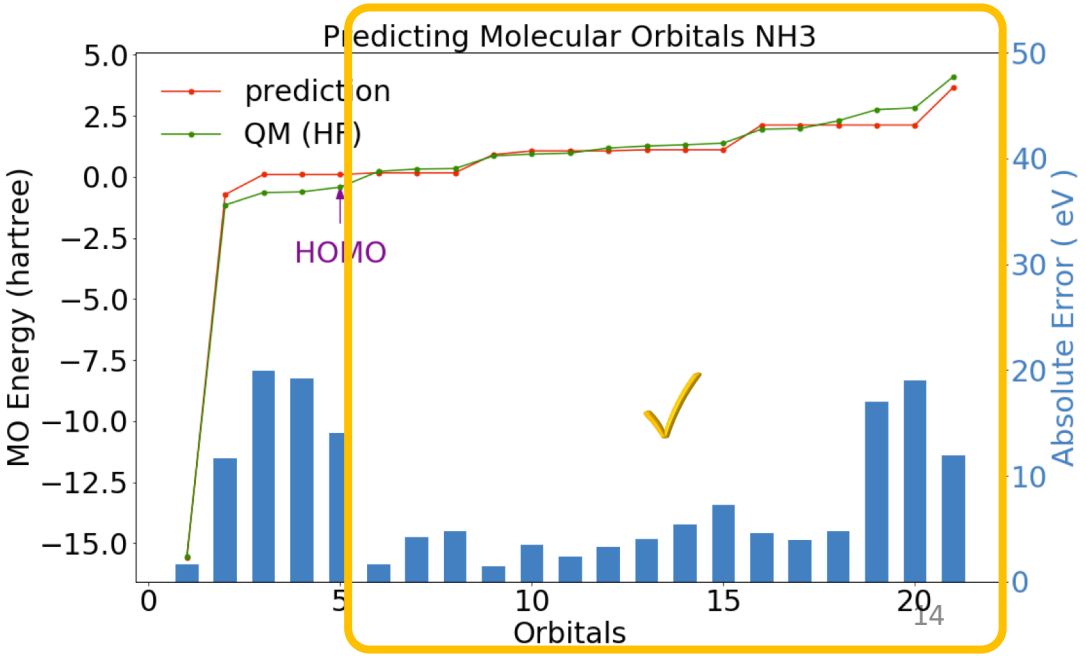
Sort



rt

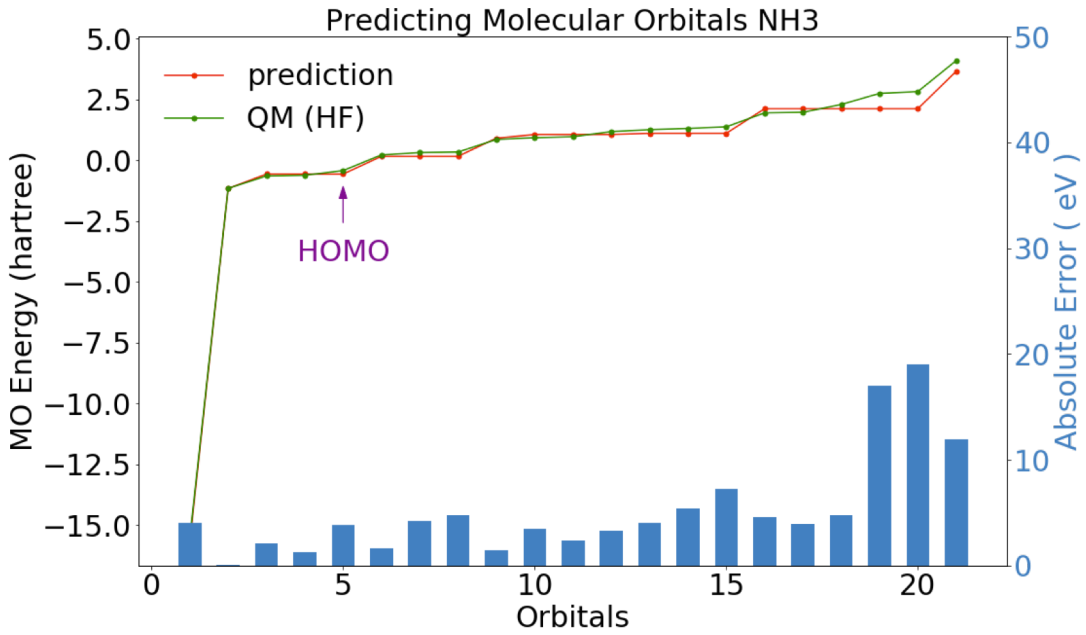


rt



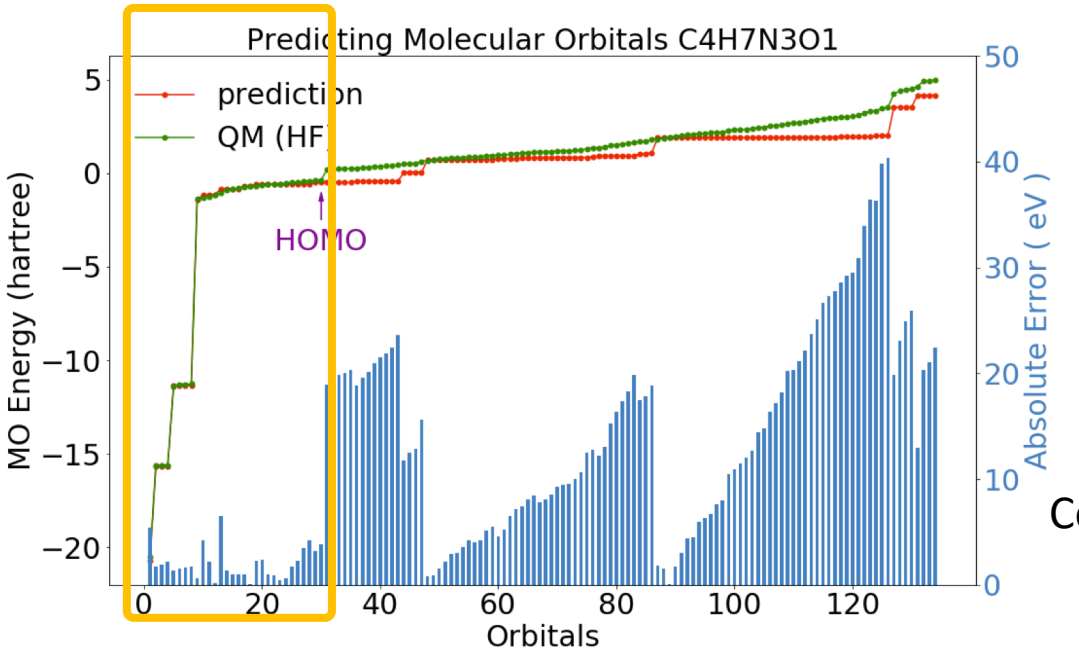
Combine

Base Line

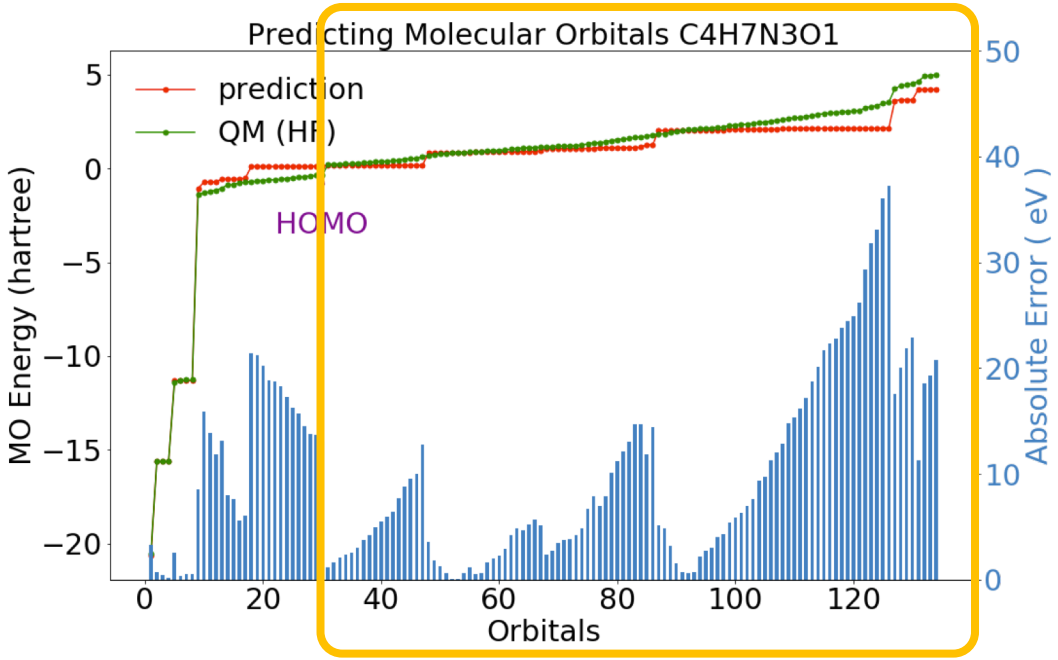


Prediction:
Correction + baseline
(correction from neural network)

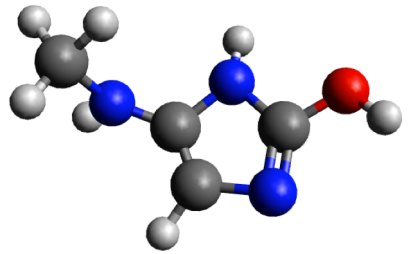
Atomic alpha orbitals



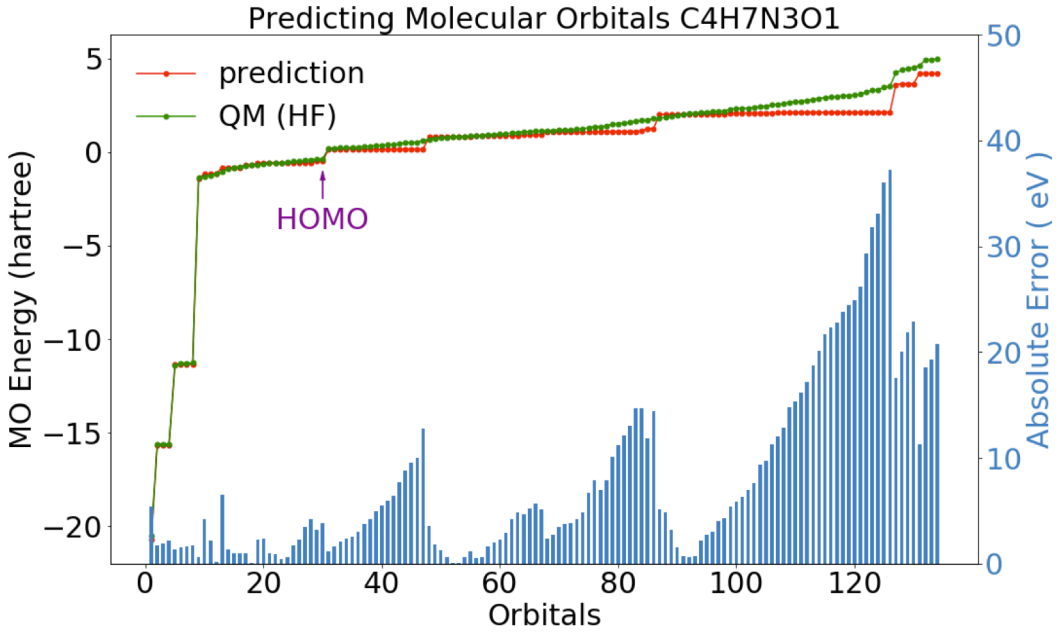
Atomic beta orbitals



Combine



$C_4H_7N_3O_1$



Molecular Orbital Model

Basis set: 6-31G*

Input: coordinates & species

Each Atom is represented by a fixed-size Atomic Environment Vector (AEV)

Extract features from AEV by different Atomic network

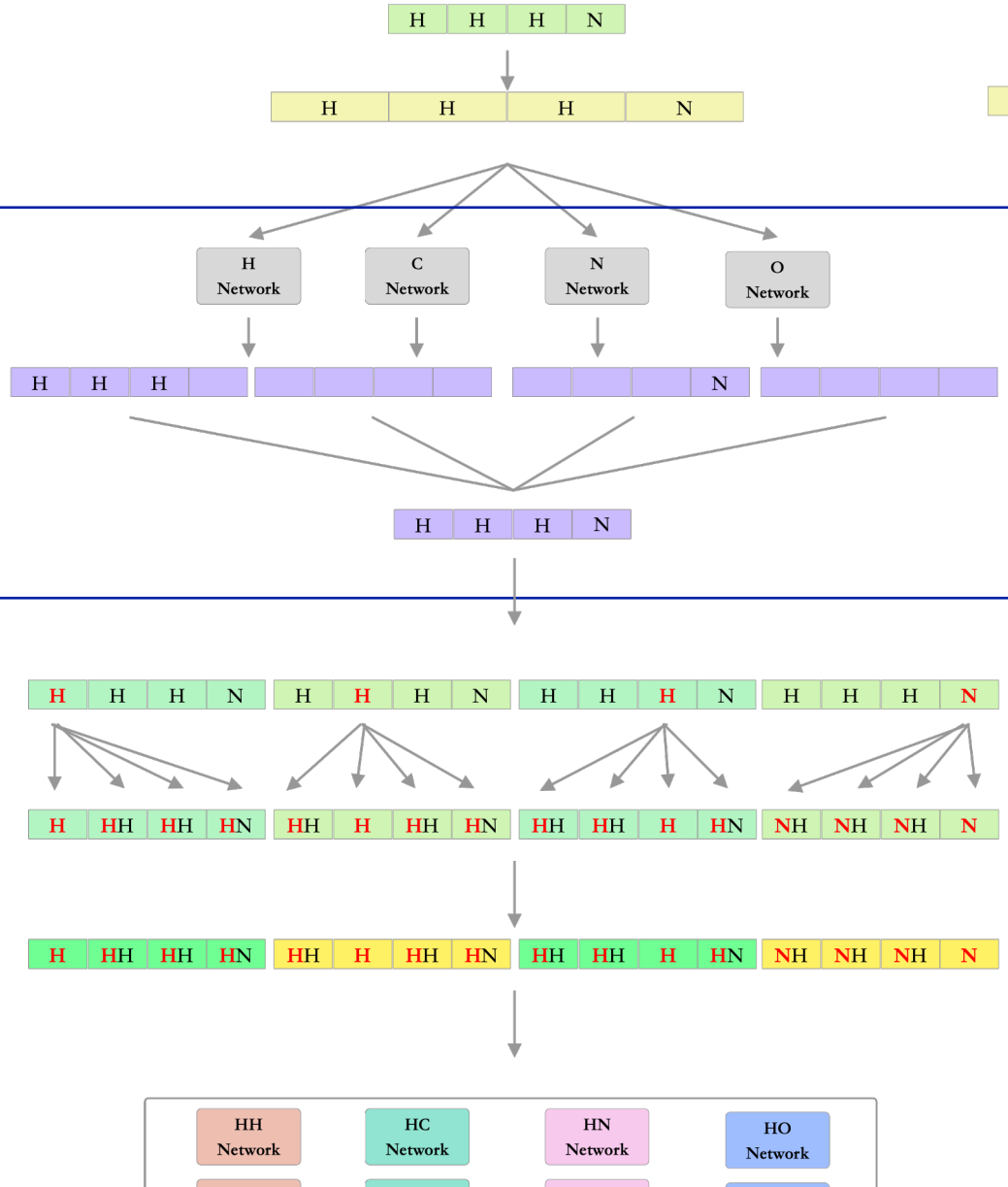
Reduced AEV

Select atom pairs

Dyadics of each pair

2 inputs —> 1 input

$$\mathbf{ab} = \mathbf{ab}^{\mathrm{T}} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} \begin{pmatrix} b_1 & b_2 & \cdots & b_N \end{pmatrix}$$



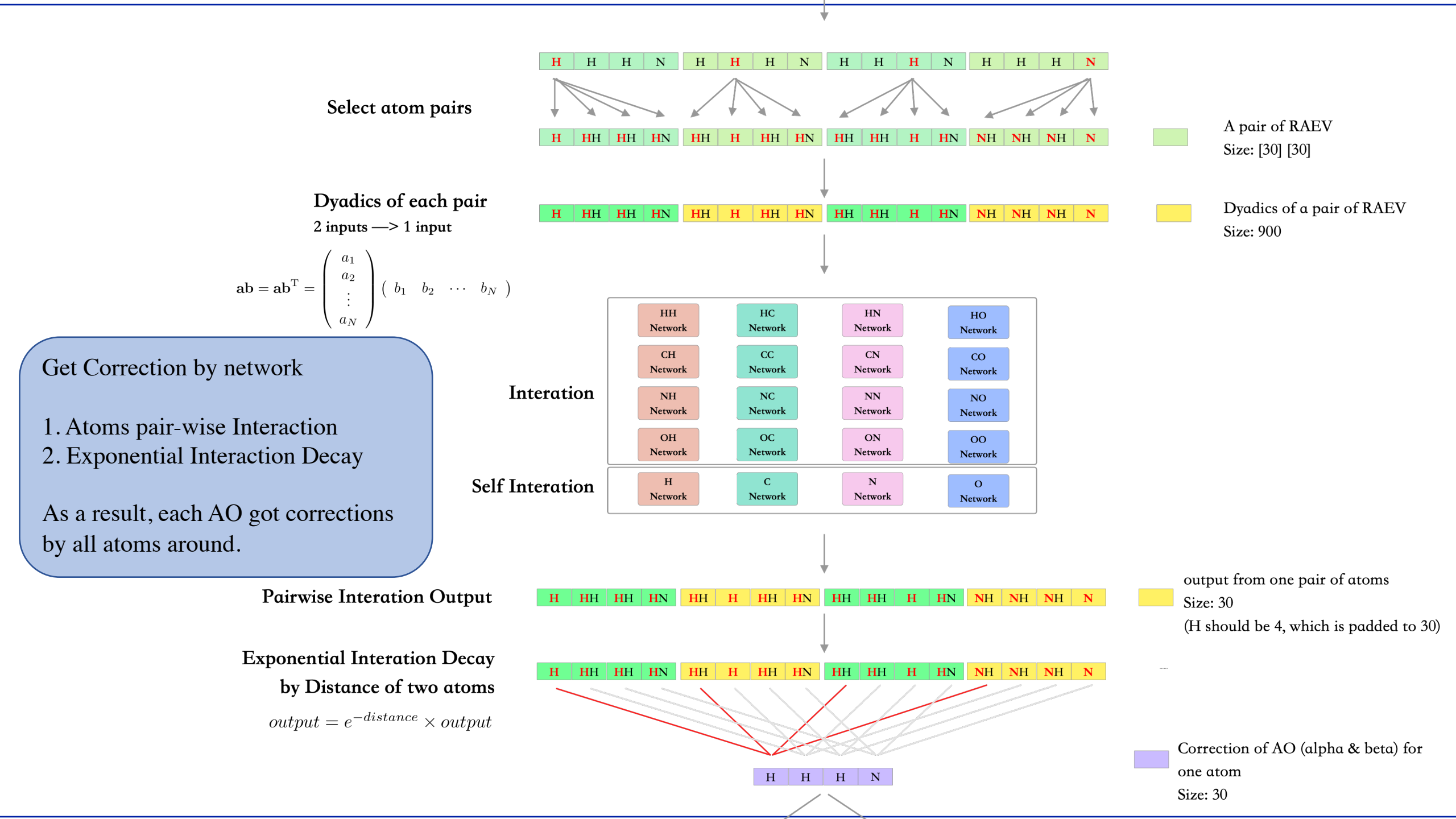
Coordinates and species
coordinates size: 3 (x, y, z)
species size: 1

AEV for 1 Atom
Size: 384 (Radial: 64 + Angular: 320)

RAEV (Reduced AEV) for 1 Atom
Size: 30

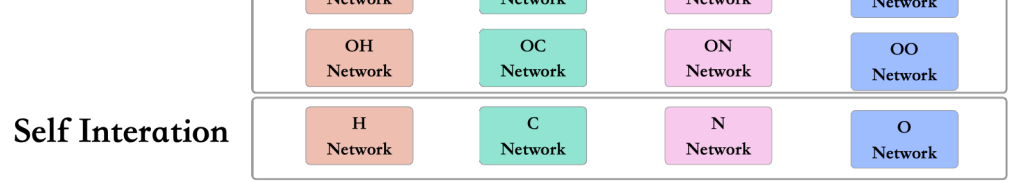
A pair of RAEV
Size: [30] [30]

Dyadics of a pair of RAEV
Size: 900

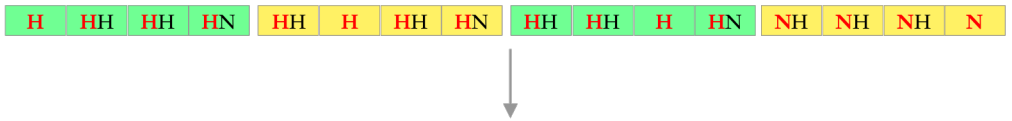

Select atom pairs
Dyadics of each pair
2 inputs —> 1 input
$\mathbf{ab} = \mathbf{ab}^{\mathrm{T}} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} \begin{pmatrix} b_1 & b_2 & \cdots & b_N \end{pmatrix}$
Get Correction by network
1. Atoms pair-wise Interaction
2. Exponential Interaction Decay
As a result, each AO got corrections by all atoms around.
Interation
HH Network
HC Network
HN Network
HO Network
CH Network
CC Network
CN Network
CO Network
NH Network
NC Network
NN Network
NO Network
OH Network
OC Network
ON Network
OO Network
Self Interation
H Network
C Network
N Network
O Network
Pairwise Interation Output
Exponential Interation Decay
by Distance of two atoms
$output = e^{-distance} \times output$
A pair of RAEV
Size: [30] [30]
Dyadics of a pair of RAEV
Size: 900
output from one pair of atoms
Size: 30
(H should be 4, which is padded to 30)
Correction of AO (alpha & beta) for one atom
Size: 30

1. Atoms pair-wise Interaction
2. Exponential Interaction Decay

As a result, each AO got corrections by all atoms around.



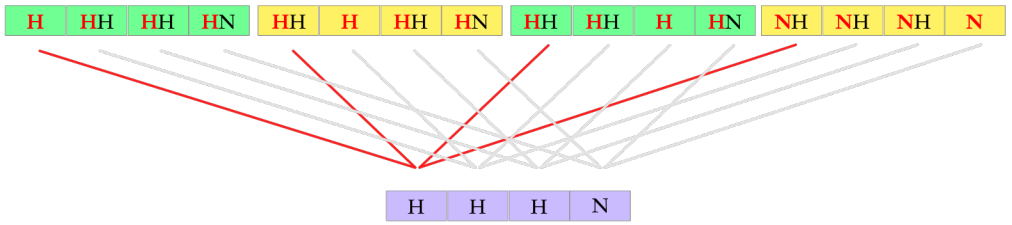
Pairwise Interation Output



output from one pair of atoms
Size: 30
(H should be 4, which is padded to 30)

Exponential Interation Decay by Distance of two atoms

$$output = e^{-distance} \times output$$



Correction of AO (alpha & beta) for one atom
Size: 30

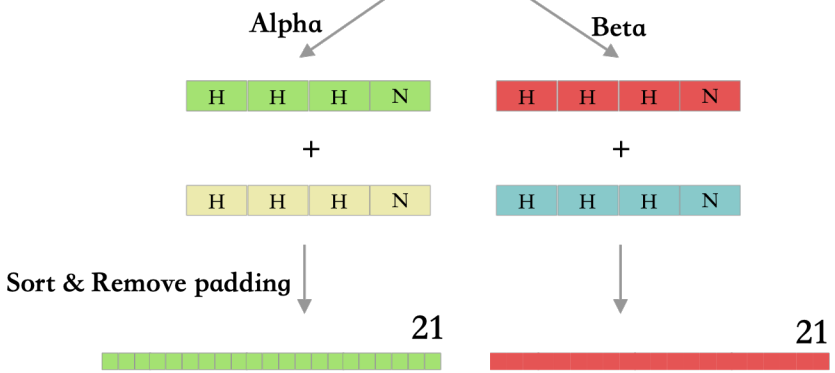
Get a variable-length final output

1. Base energies + Correction by network
2. Sort
3. Combine

AO Correction by ANI

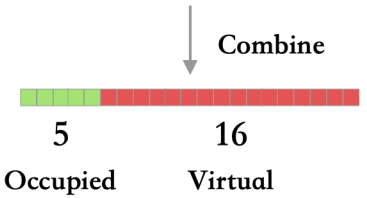
+

AO base Energy



Corrected AO

Correction of AO (alpha or beta) for one atom
Size: 15



Output: Molecular Orbital

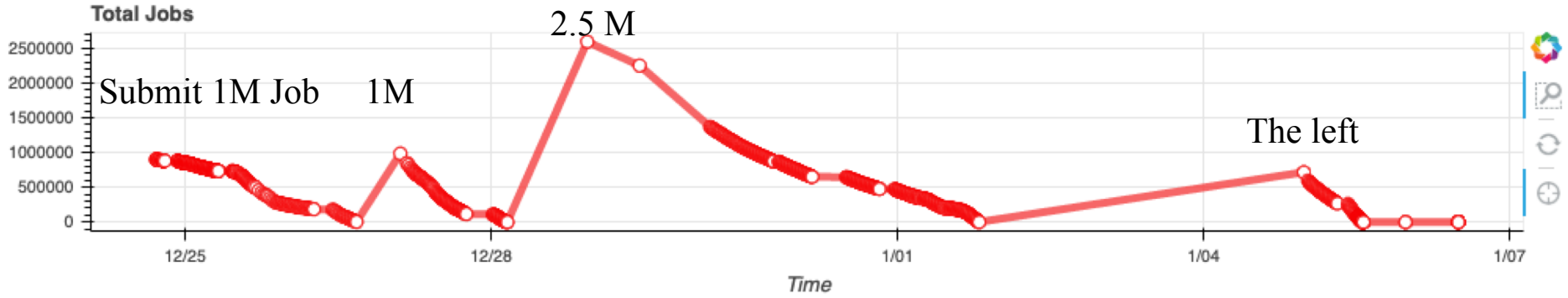
One Molecular Orbital Energy
Size: 1

Total parameters: 7,171,582

ANI: 326,660

Dataset

- 4.1 M conformations (837 molecules)
  - 84.2 % of ANI-1x dataset (4.9 M conformations, 3,114 molecules, CHNO)
  - Number of electrons less than 71
  - 4 ~ 25 atoms, non-H atom 1 ~ 10
- HF / 6-31G(d) using PSI4 package
- TACC Frontera within 10 days (75 Nodes (each has 56 threads))
  - Tool: HTRQ by Roman Zubatyuk (for ORCA)
  - Developed a PSI4 version
  - Integrate Redis Queue, Mongo Database

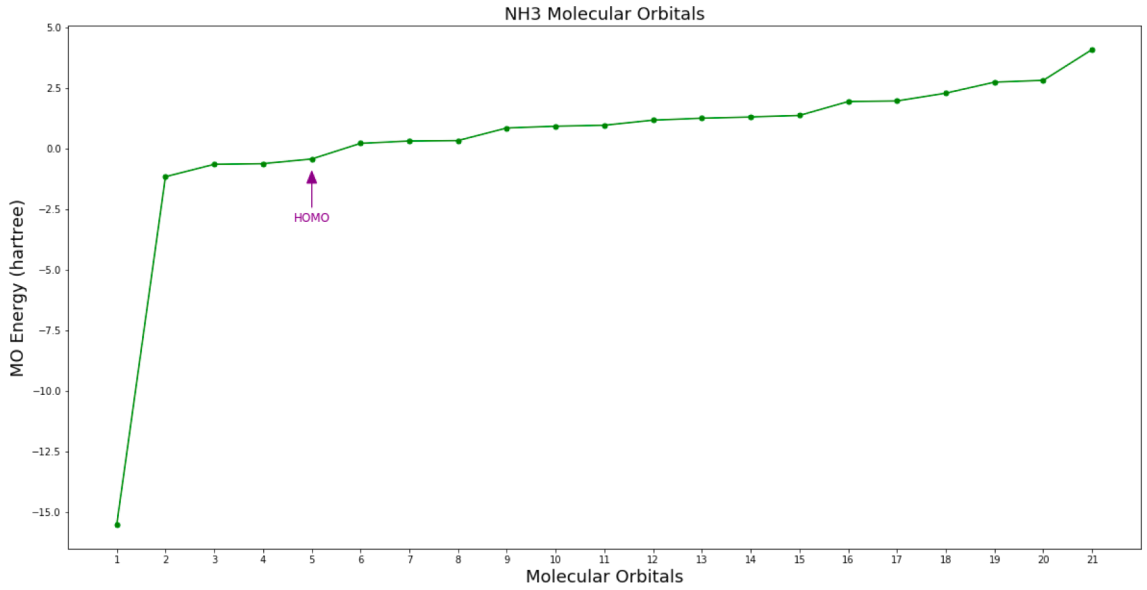


Result

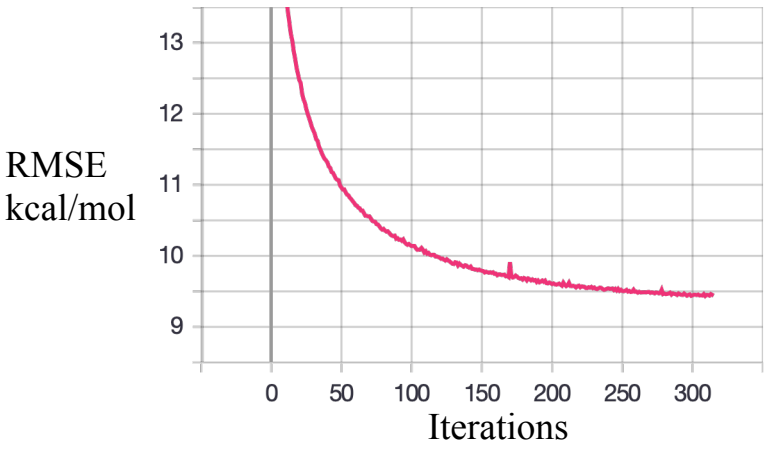
- Training vs Validation: 9:1
- Batch size: 1000
- Optimizer: ADAM
- Framework: PyTorch
- Package: TorchANI (for AEV)

- Loss function:
  1. MSE per MO for all orbitals — loss_all
  2. MSE per MO for minimal orbitals
     +
     0.1 (MSE per MO for the left orbitals) — loss_mini

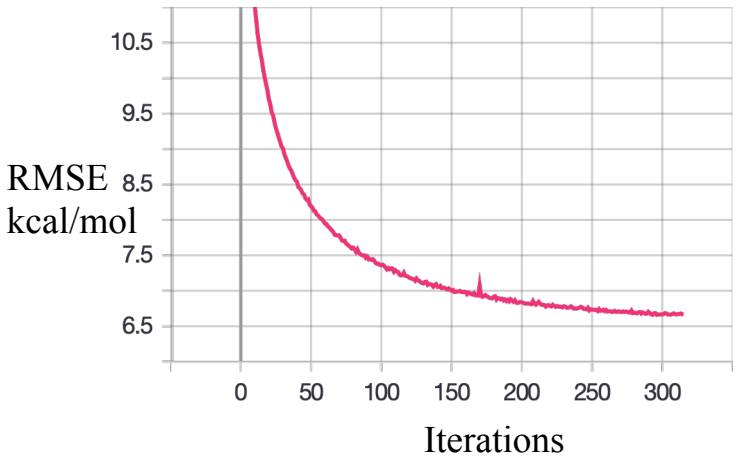
- Two seperate training (100h on 1 single GPU)
  1. Only training on loss_all
  2. First 100 iteration train on loss_all, then change to loss_mini



Validation RMSE for all



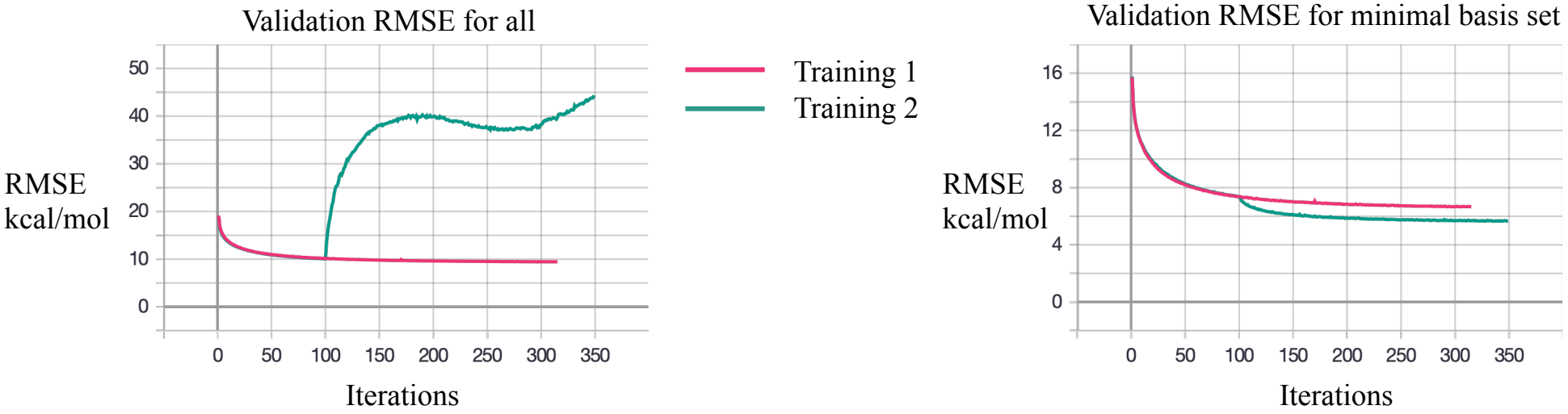
Validation RMSE for minimal basis set



Training 1:
Only training on loss_all

Validation RMSE in kcal/mol

	RMSE_all	RMSE_mini
Training 1	9.4405	6.6611



Validation RMSE in kcal/mol

Training 1:
Only training on loss_all

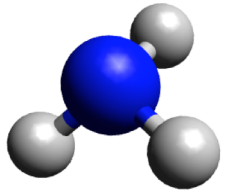
	RMSE_all	RMSE_mini
Training 1	9.4405	6.6611

Training 2:
First 100 iteration train on loss_all,
then change to loss_mini

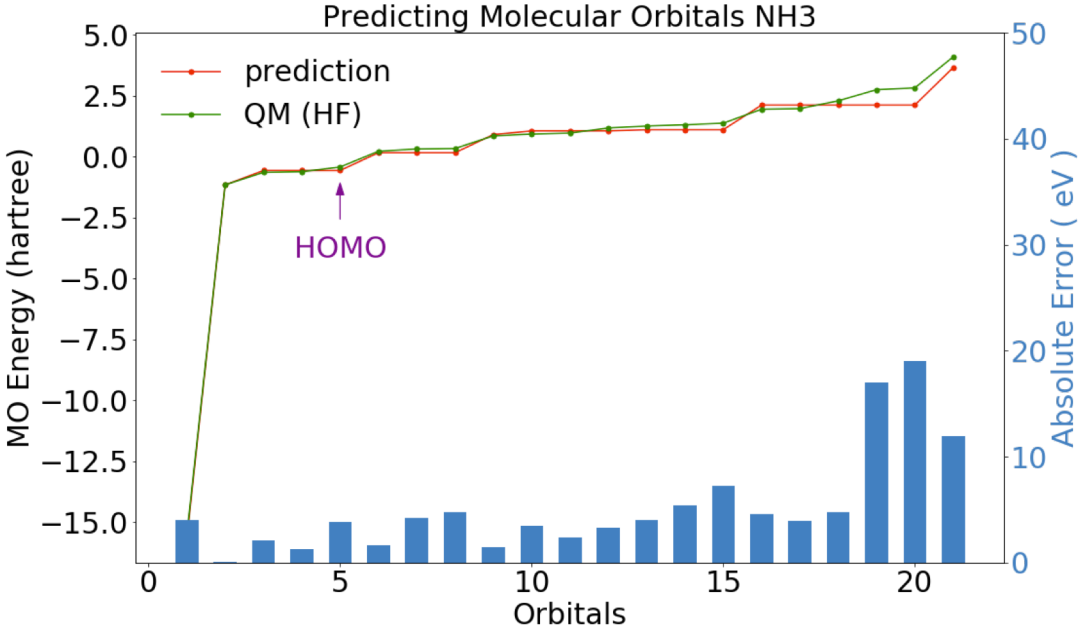
	RMSE_all	RMSE_mini
Training 2	44.3752	5.6452

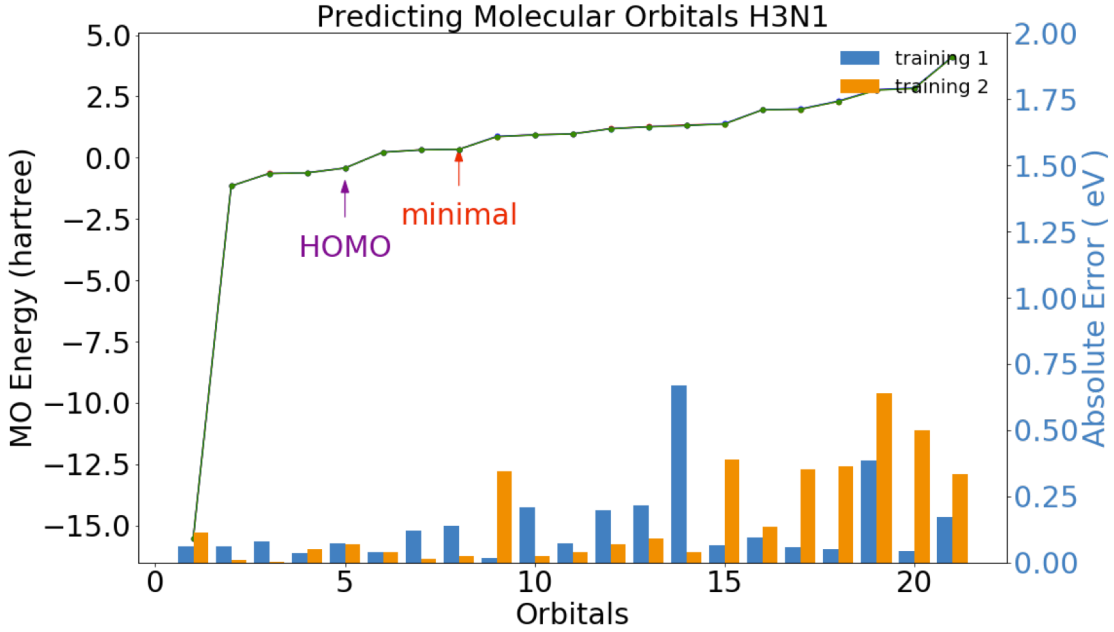
Base Line

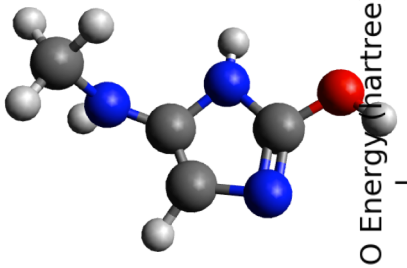
Prediction



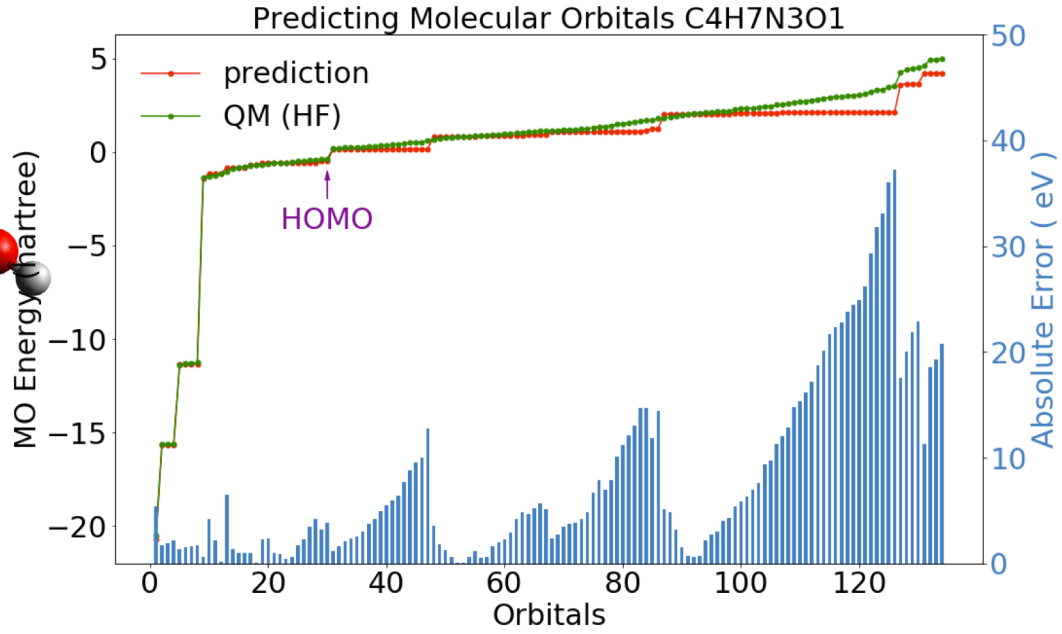
NH3

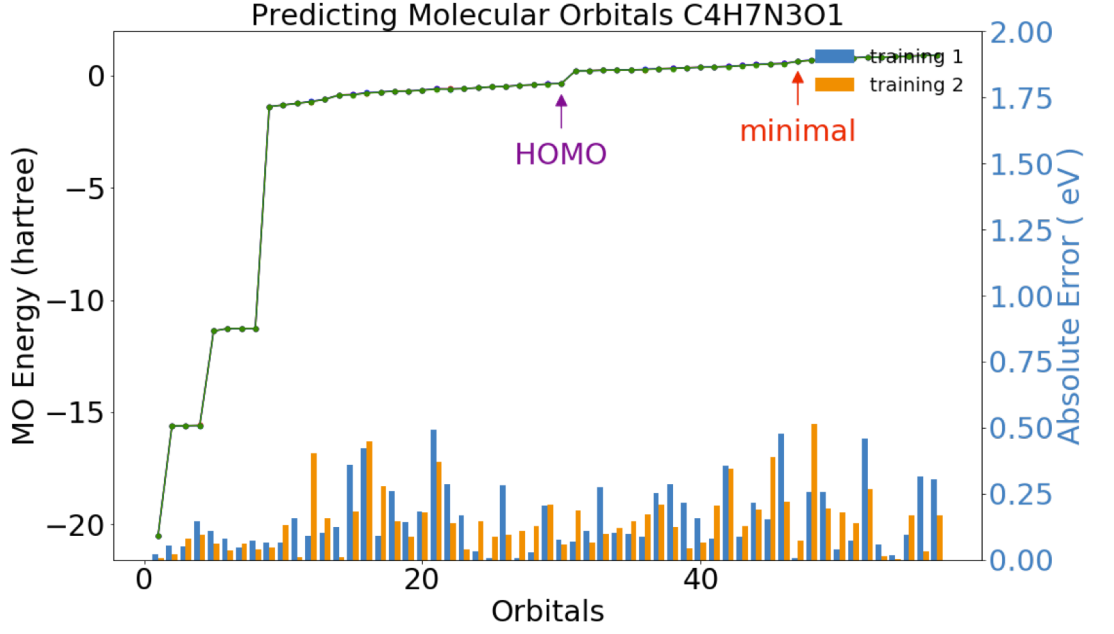






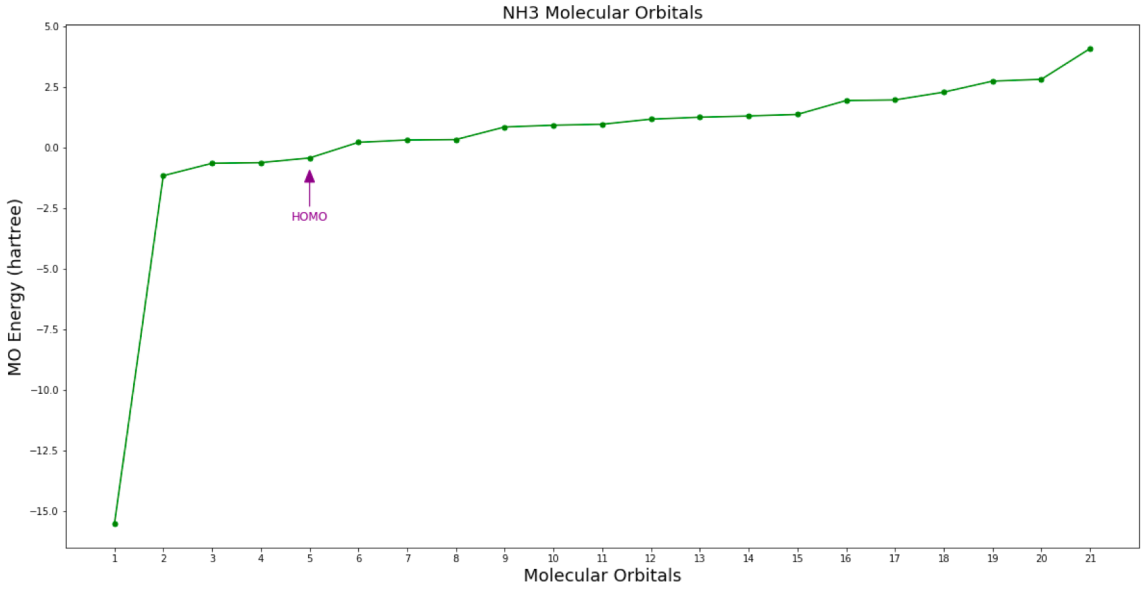
$C_4H_7N_3O_1$





Future work

- Design of the model (physical meaning)
- Optimization
  - Loss function:
    - Take gap between orbitals into account
  - Learning rate decay
  - Model Architecture
  - Try DFT dataset



Thanks

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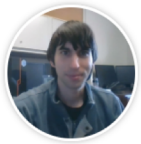

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