Entrenamientos Destacados

# Mejor Energía

Este entrenamiento tiene como target la energía total menos la atómica.

Configuración relevante:

batch\_size: 32

cutoff\_upper: 6.35

derivative: False

inference\_batch\_size: 4

max\_num\_neighbors: 140

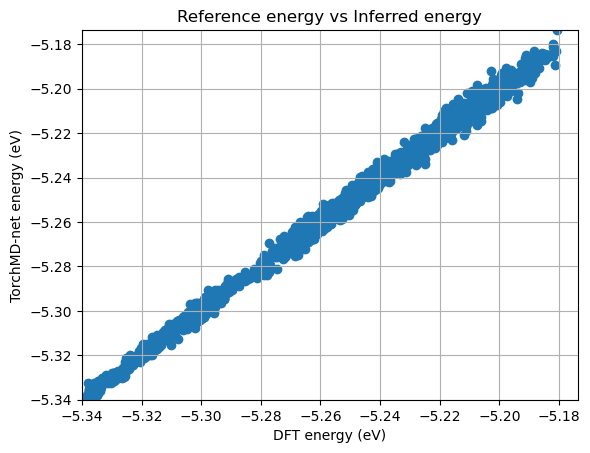
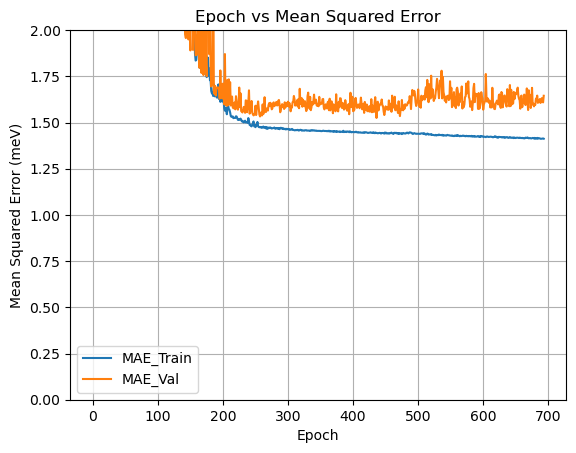
num\_epochs: 1000

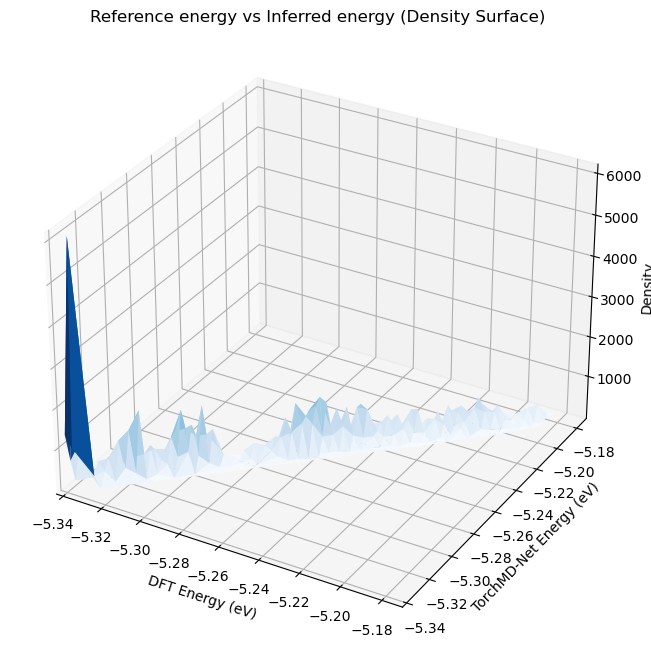
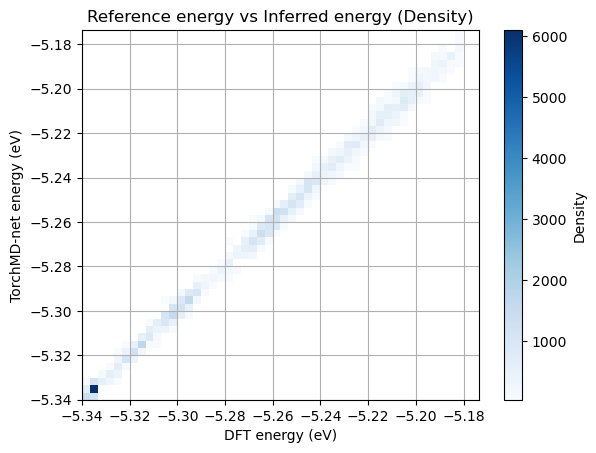
seed: 42

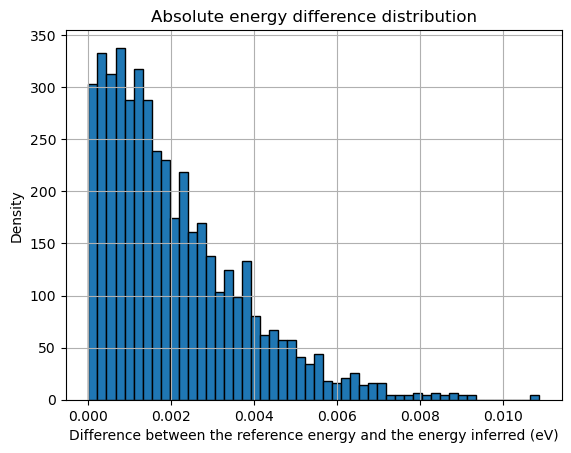
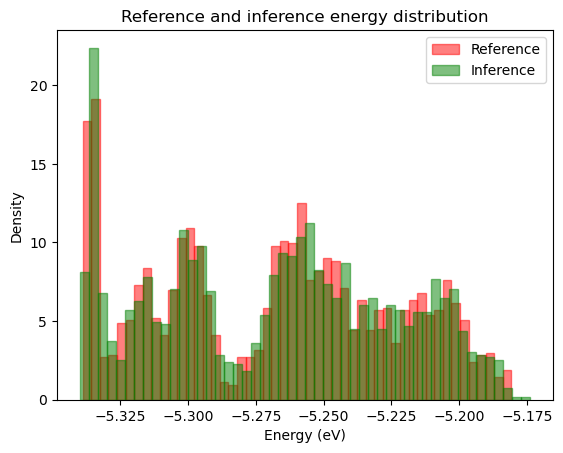
test\_size: 0.1

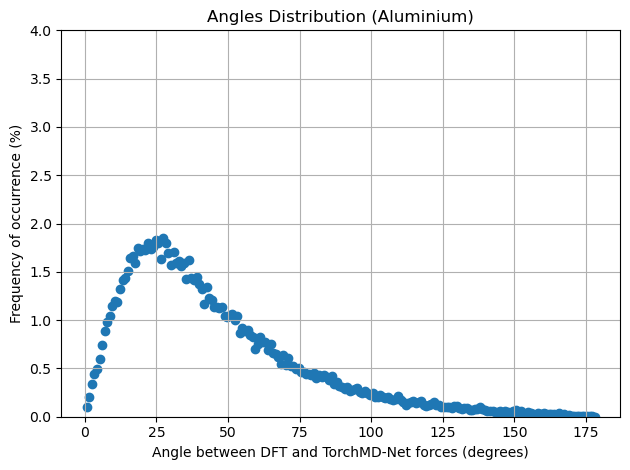
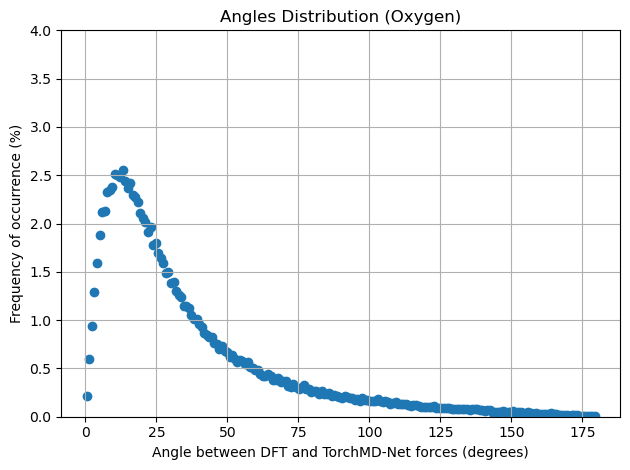
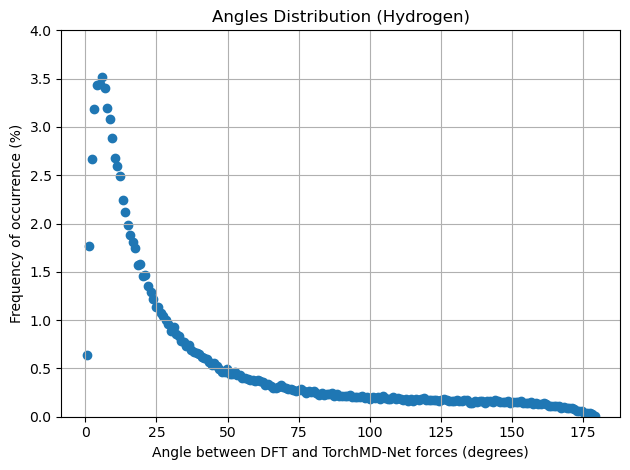
train\_size: 0.81

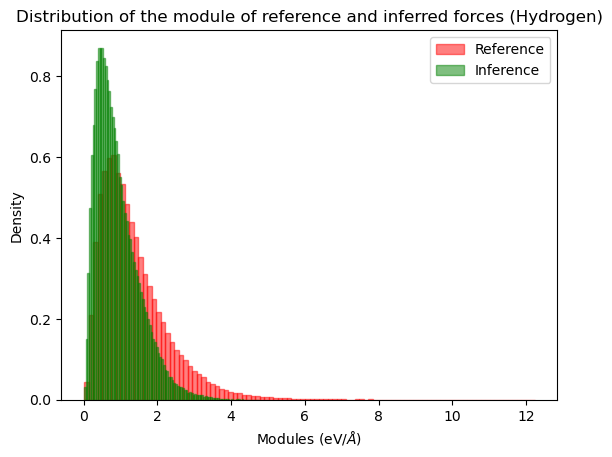
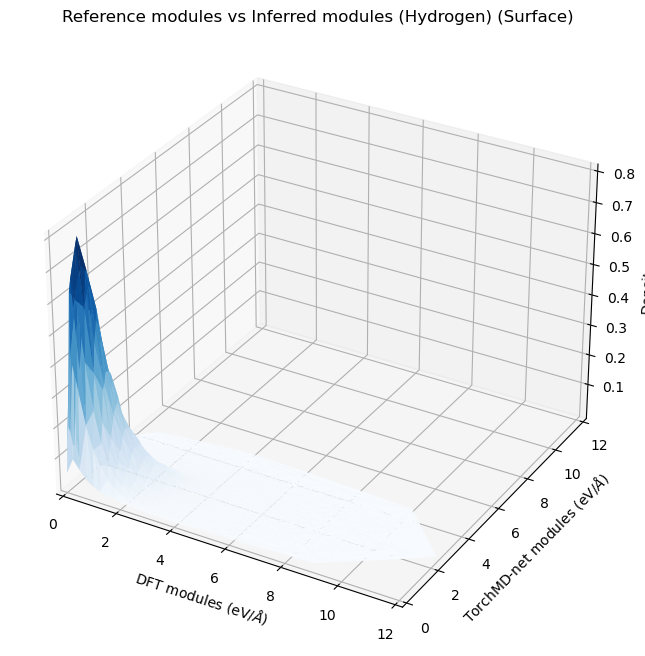
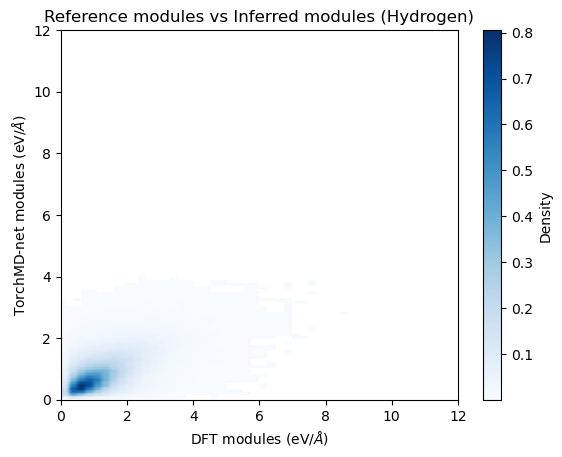
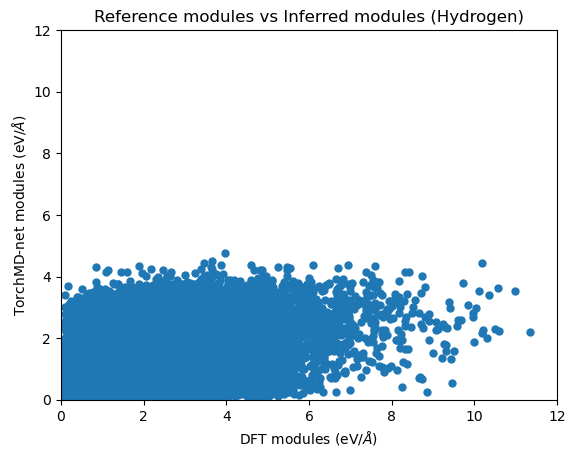
val\_size: 0.09

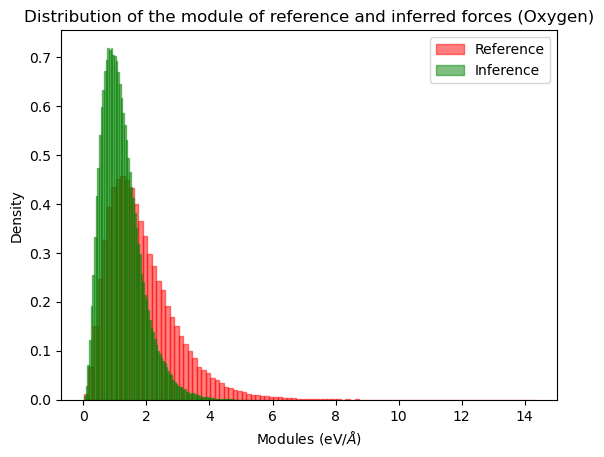
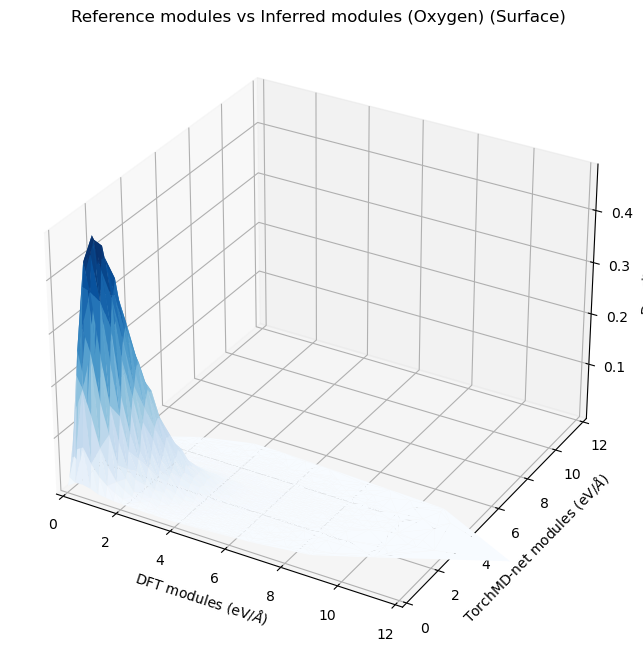
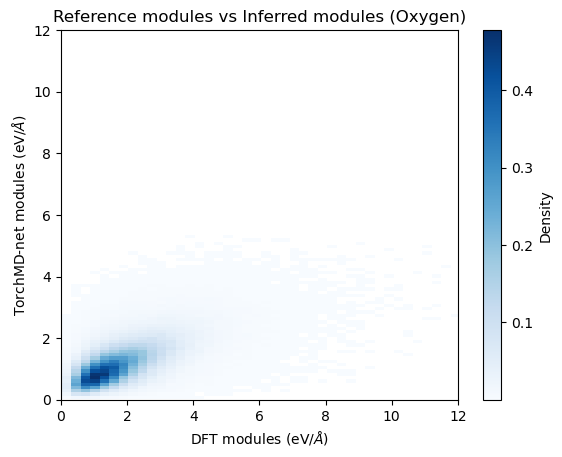
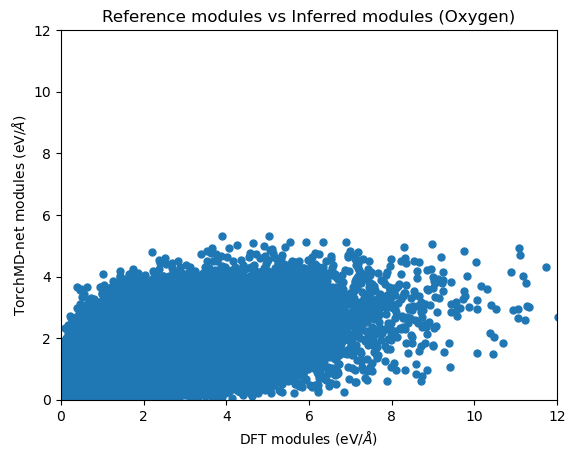


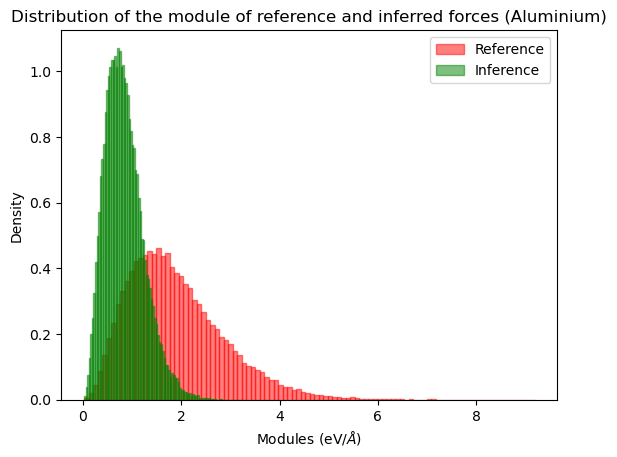
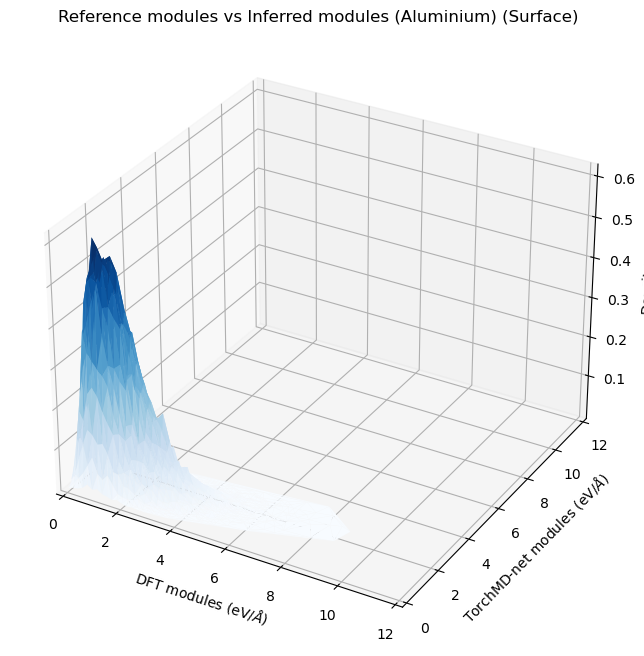
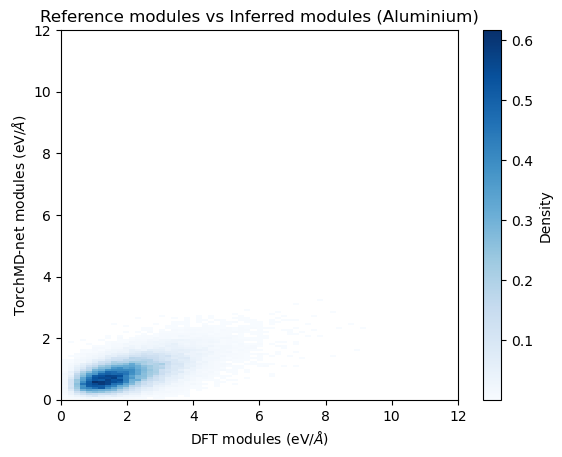
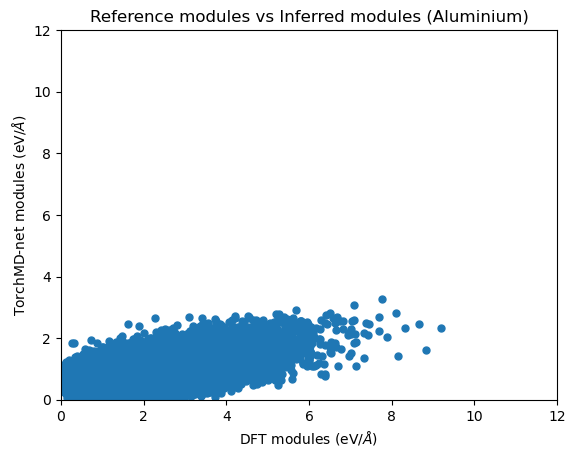












# 

# Mejor Fuerza

La duración del entrenamiento es de 7 horas, 5 minutos y 28 segundos.

Configuración relevante:

batch\_size: 32

cutoff\_upper: 6.35

derivative: True

y\_weight: 0.0001

neg\_dy\_weight: 1.0

inference\_batch\_size: 4

max\_num\_neighbors: 140

num\_epochs: 1000

seed: 42

test\_size: 0.1

train\_size: 0.81

val\_size: 0.09

