

# Relaxing the system

**Script:** relaxation.py

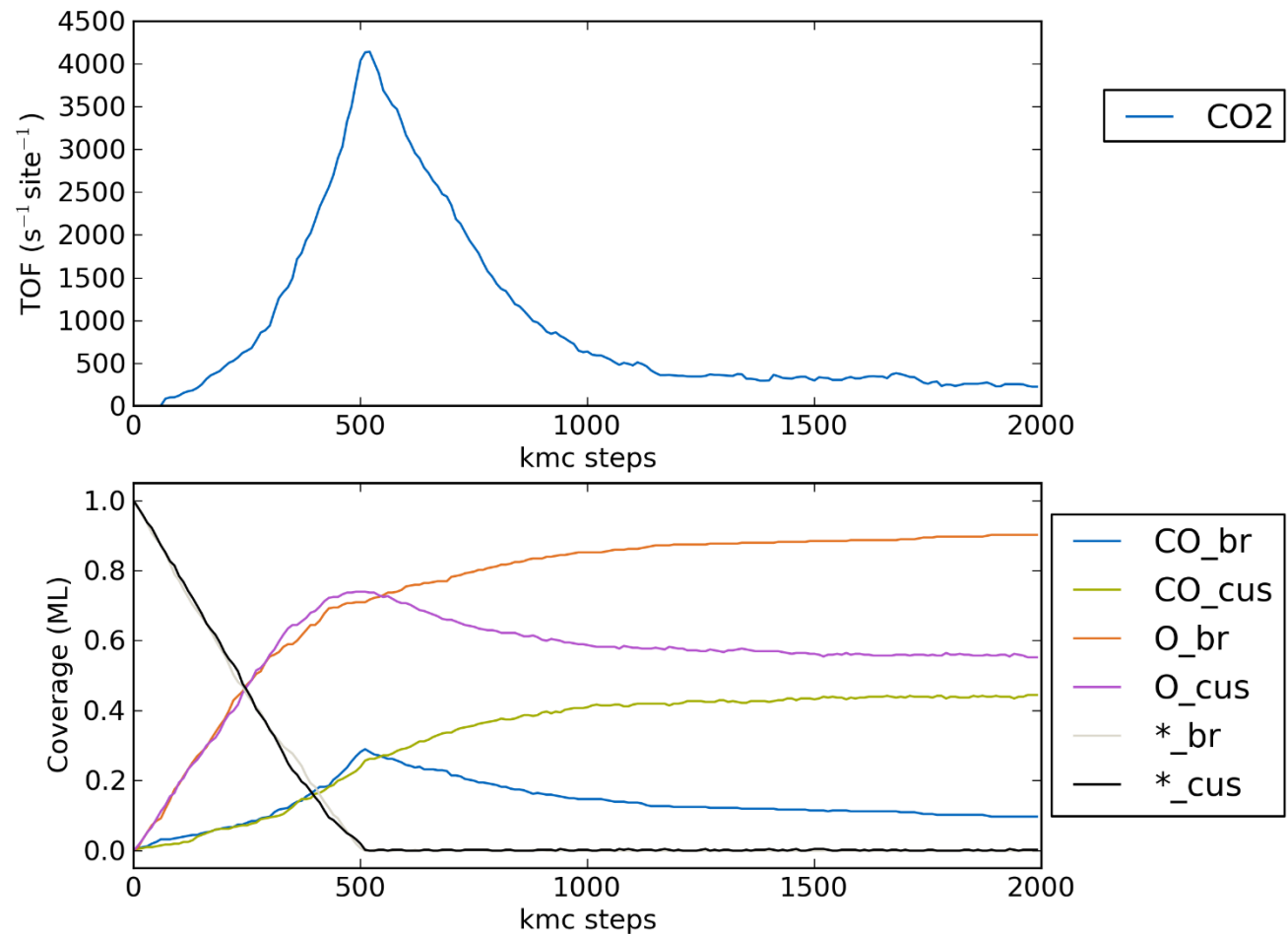
$T = 450 \text{ K}$

$p(\text{CO}) = 1 \text{ bar}$

$p(\text{O}_2) = 1 \text{ bar}$

**Initial state:** clean

**kMC steps:** 2000



# Relaxing the system

**Script:** relaxation.py

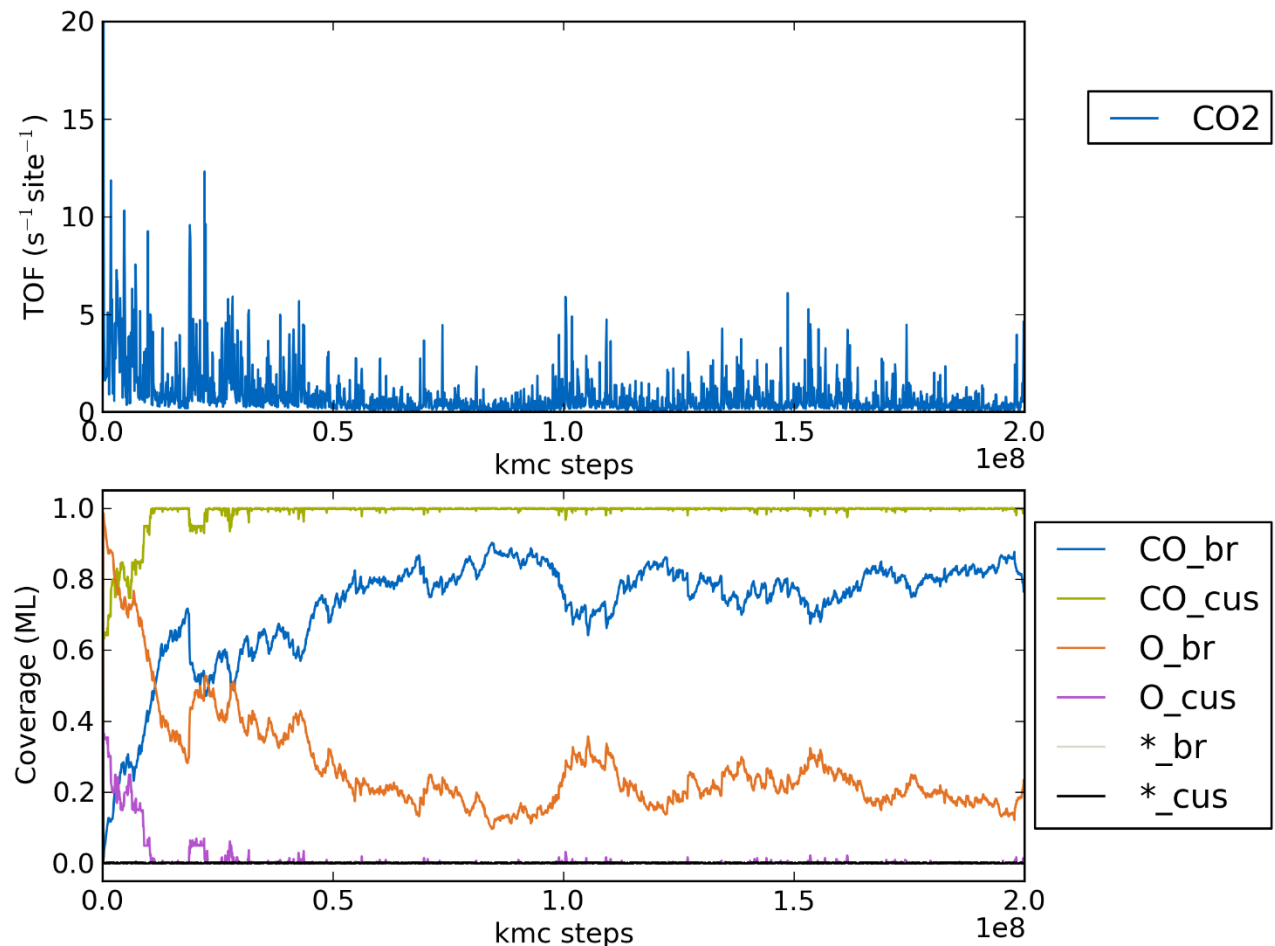
$T = 450 \text{ K}$

$p(\text{CO}) = 1 \text{ bar}$

$p(\text{O}_2) = 1 \text{ bar}$

**Initial state:** clean

**kMC steps:**  $2 \cdot 10^8$



# Preparing the initial state

## **Modify occupation of single site:**

```
model.put(site=[x,y,z,model.lattice.<site>], model.proclist.<species>)
```

## **More efficient for many sites:**

```
Model._put(...)  
model._put(...)  
...  
model._adjust_database()
```

**Script:** relaxation.py

Uncomment lines 16-19

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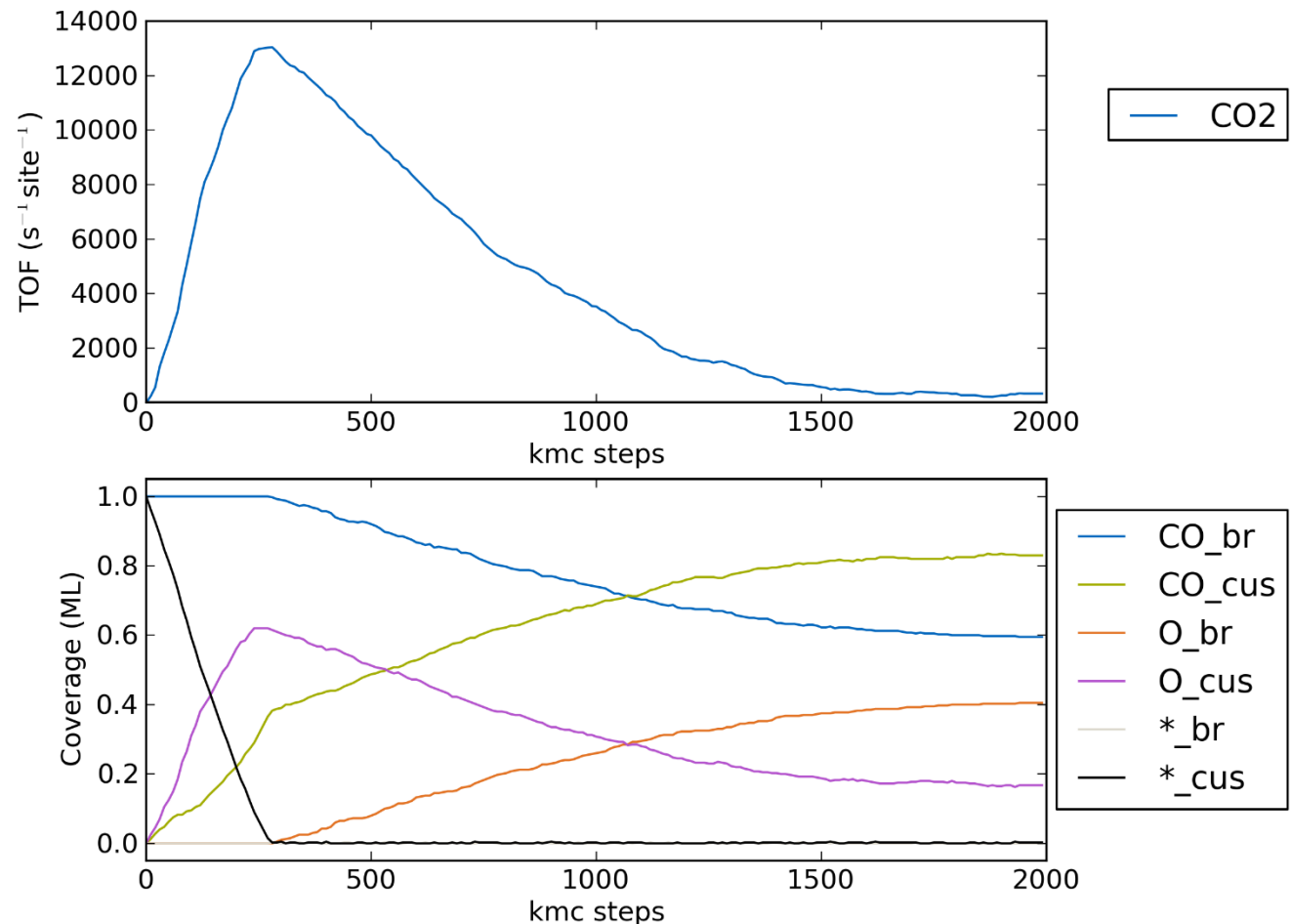
$T = 450 \text{ K}$

$p(\text{CO}) = 1 \text{ bar}$

$p(\text{O}_2) = 1 \text{ bar}$

**Initial state:** CO@br

**kMC steps:** 2000



# Relaxing the system

**Script:** relaxation.py

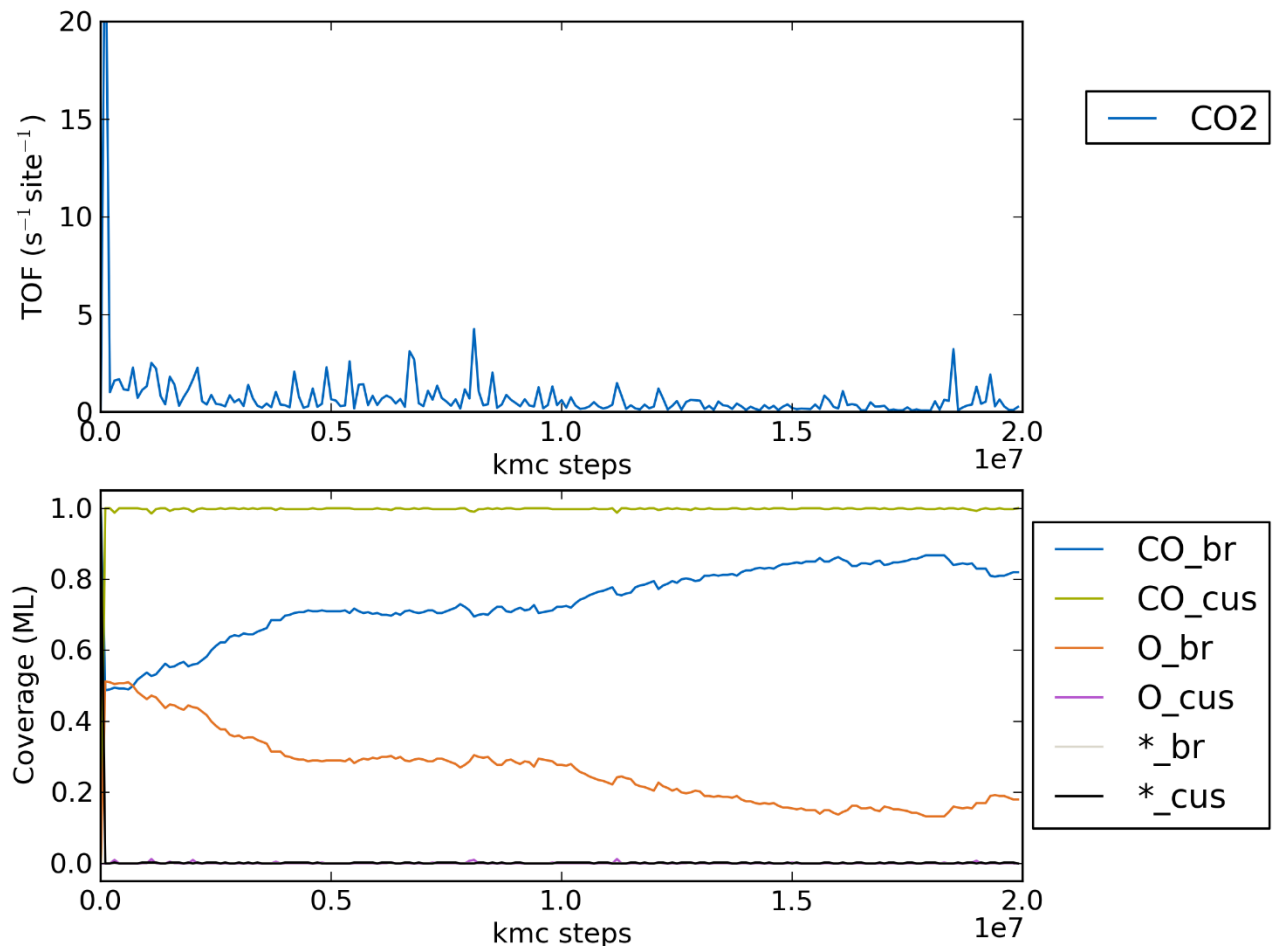
$T = 450 \text{ K}$

$p(\text{CO}) = 1 \text{ bar}$

$p(\text{O}_2) = 1 \text{ bar}$

**Initial state:** CO@br

**kMC steps:**  $2 \cdot 10^7$



# Relaxing the system

**Script:** relaxation.py

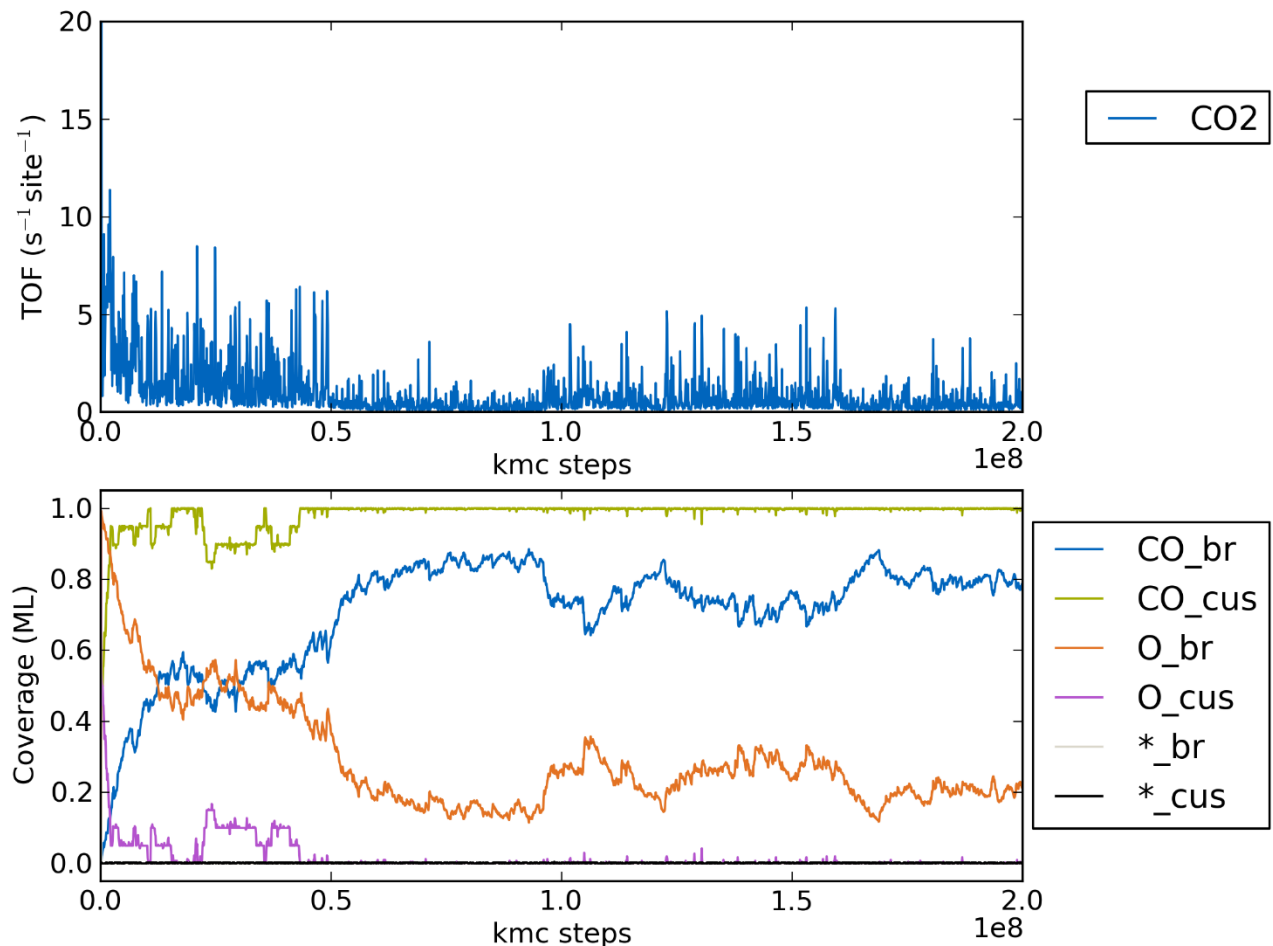
$T = 450 \text{ K}$

$p(\text{CO}) = 1 \text{ bar}$

$p(\text{O}_2) = 1 \text{ bar}$

**Initial state:** O@cus

**kMC steps:**  $2 \cdot 10^8$



# Random initial state from guess coverages

## Script:

relaxation\_random.py

$T = 450 \text{ K}$

$p(\text{CO}) = 1 \text{ bar}$

$p(\text{O}_2) = 1 \text{ bar}$

**Initial state:** random  
based on known  
coverages.

**kMC steps:**  $2 \cdot 10^8$

