

# MOSP: Multi-scale Operando Simulation Package

The screenshot displays the MOSP software interface, which is divided into two main sections: MSR (Multi-scale Simulation) and KMC (Kinetic Monte Carlo Simulation).

**MSR Section:**

- Initial structure:** MSR Structure (selected) or Read from file.
- Total steps:** [Input field] **Record interval:** [Input field]
- Size of the Simulation box(Å):** x [Input field] y [Input field] z [Input field]
- Diffusion barrier(eV):** gas1 [Input field] gas2 [Input field]
- Sticking coefficient:** Gas1: -- on edge [Input field] on face [Input field]  
Gas2: -- on edge [Input field] on face [Input field]
- Coefficient of E<sub>ads</sub>(gc):** Gas1: -- a [Input field] b [Input field]  
Gas2: -- a [Input field] b [Input field]
- Coefficient of BEP relation:** a [Input field] b [Input field]
- Average lateral interaction(eV):** gas1-gas1: [Input field]  
gas1-gas2: [Input field]  
gas2-gas2: [Input field]

**KMC Section:**

- Element:** [Input field] **Lattice constant(Å):** [Input field] **Crystal structure:** FCC (dropdown)
- Pressure(Pa):** [Input field] **Temperature(K):** [Input field] **Radius(Å):** [Input field]
- Gas parameters table:**

Name	Partial Pressure(%)	Gas Entropy(eV/T)	Adsorption type
Gas1	[Input field]	[Input field]	Associative (dropdown)
Gas2	[Input field]	[Input field]	Associative (dropdown)
Gas3	[Input field]	[Input field]	Associative (dropdown)
- Number of faces:** 3 (Add/Remove buttons)
- Surface energy table:**

Index	Surface energy(eV/Å <sup>2</sup> )	E <sub>ads</sub> (eV)	S <sub>ads</sub> (eV/T)	Lateral interaction(eV)
[Input field]	[Input field]	unset	unset	unset
[Input field]	[Input field]	unset	unset	unset
[Input field]	[Input field]	unset	unset	unset

Buttons: Load, Save, run (for both MSR and KMC sections).

Fig 1. Graphic Interface of MOSP Software

## MSR :

### 1. Basic Parameters:

- [Element]: Set the metal type.
- [Lattice constant]: Set the lattice constant (unit: Å).
- [Crystal structure]: Set the crystal structure. Only FCC and BCC is supported in current version.
- [Pressure]: Set the total pressure of the gas environment (unit: Pascal).
- [Temperature]: Set the temperature of the environment (unit: Kelvin).
- [Radius]: Set the radius of the metal nanocluster (unit: Å).

### 2. Parameters of gases:

One to three gases can be selected as the gas environment. Each gas contains the following parameters:

- [Name]: Set the name of gas.
- [Partial Pressure]: Set the partial pressure of gas (unit: %).
- [Gas Entropy]: Set the gas entropy of gas under 1atm (unit: eV/T). This value may be found on the NIST-JANAF website.

- [Adsorption type]: Set the adsorption type of gas. ‘Associative’ means:  $A + * \rightarrow A^*$ . And ‘Dissociative’ means:  $A_2 + 2* \rightarrow 2A^*$

### 3. Parameters of faces:

- [Index]: Miller index [hkl]
- [Surface energy]: Surface energy  $\gamma$  (unit: eV/Å<sup>2</sup>)
- [E\_ads]: Adsorption energy of each gas (unit: eV).
- [S\_ads]: Adsorption entropy of each gas (unit: eV/T).
- [Lateral interaction]: Lateral interaction between gases (unit: eV).

### 4. Example:

Load the input file Pt\_msr.txt under Path \input\Pt and run MSR module (Fig 2(a)). The configuration of Pt nanoparticle in CO/O<sub>2</sub> binary gas environment will be built and visualized (Fig 2(b)).

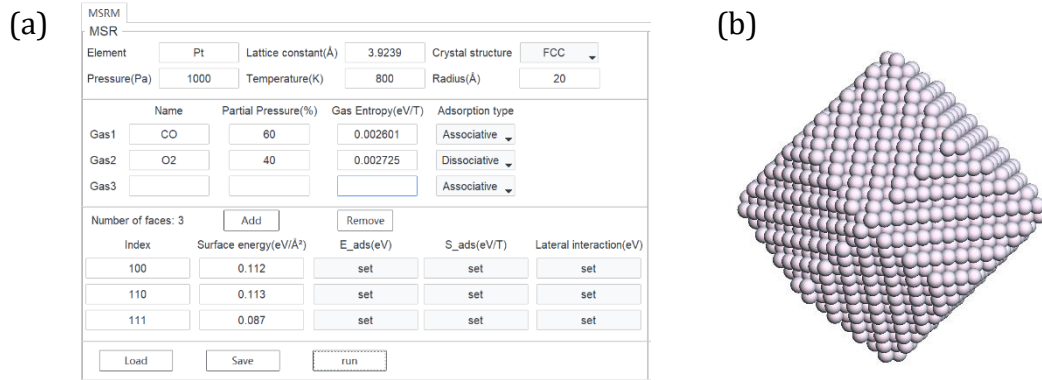


Fig 2. (a) MSR Parameters. (b) Pt nanoparticle ( $R=20$  Å) in CO/O<sub>2</sub> binary environment ( $T = 800K$ ,  $P = 1000Pa$ )

### KMC:

After the running of MSR, a nanoparticle will be built. Then you can run a Kinetic Monte Carlo simulation (KMC) based on this nanoparticle. It may take several minutes. When KMC simulation end, a result analysis window can be opened (Fig 3). Gaseous coverage and TOF trends in the simulation process will be plotted. And the event statistics in log coordinates. The catalytic activity of each site is represented by coloring the nanoparticle. The color bar from 0 to maximum is blue to red.

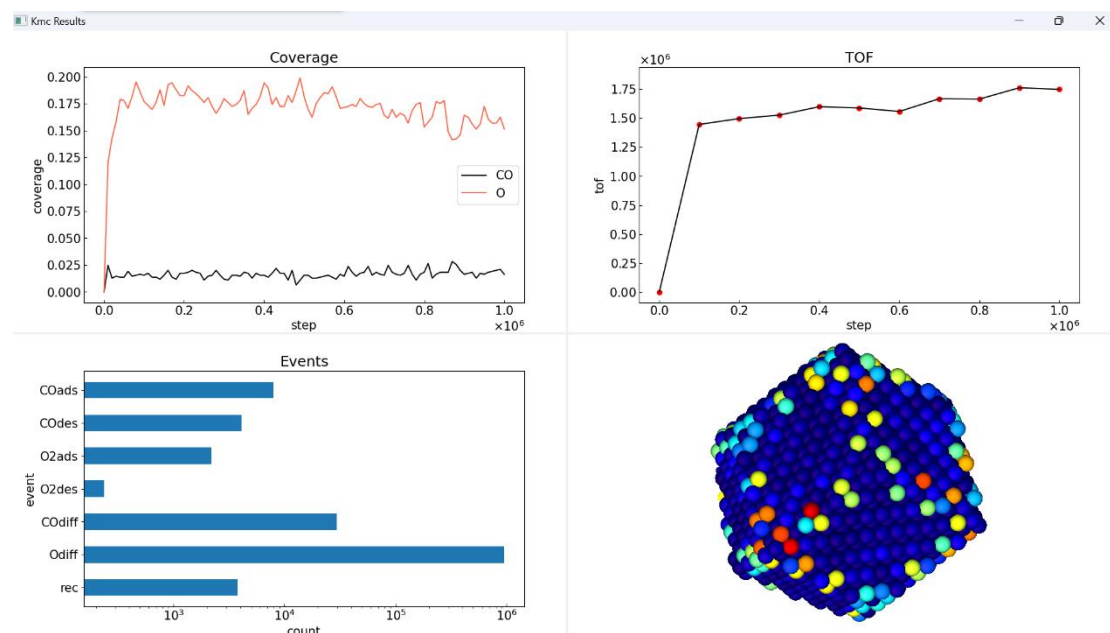


Fig 2. KMC Result analysis window