MOSP: Multi-scale Operando Simulation Package

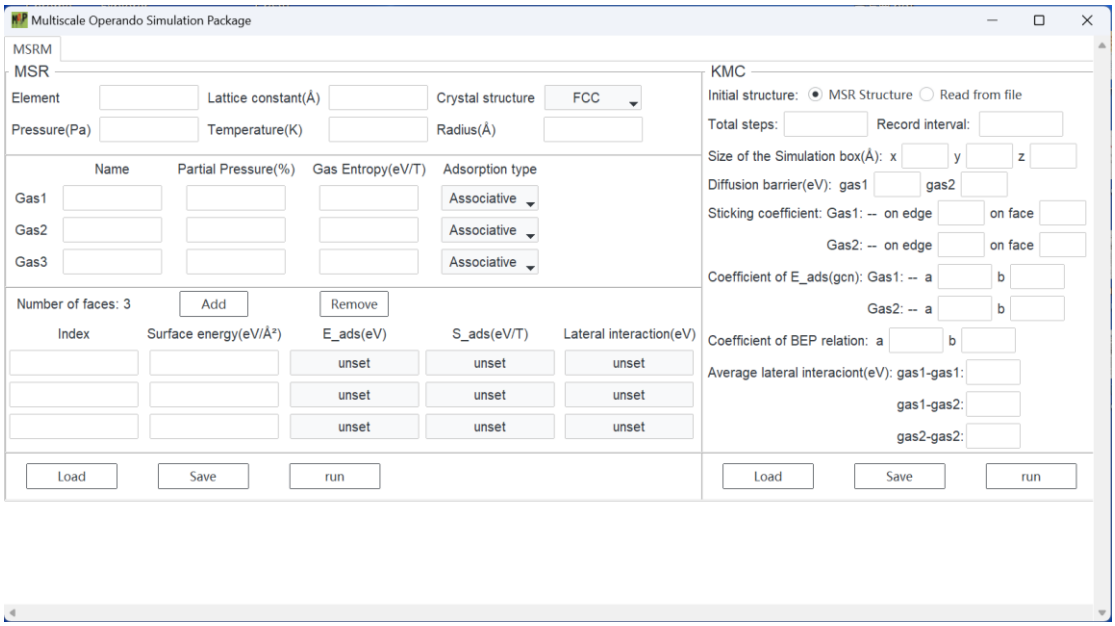


Fig 1. Graphic Interface of MOSP Software

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+ * →A*. And 'Dissociative' means: $A_2+2* \rightarrow 2A*$

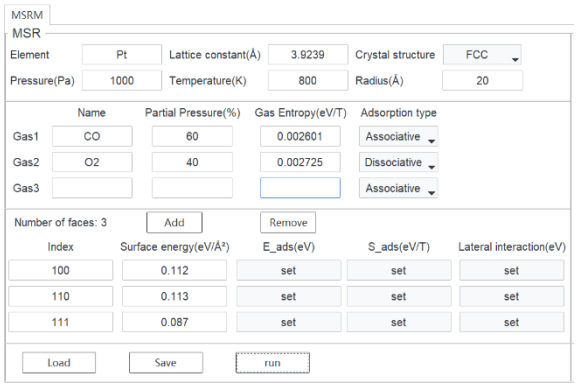
3. Parameters of faces:

- [Index]: Miller index [hkl]
- [Surface energy]: Surface energy γ (unit: eV/Å^2)
- [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/O2 binary gas environment will be built and visualized (Fig 2(b)).

(a)



(b)

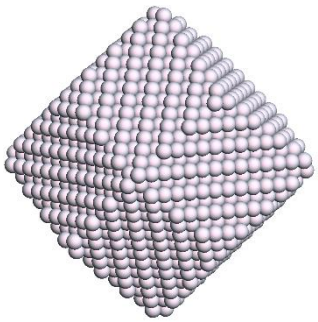


Fig 2. (a) MSR Parameters. (b) Pt nanoparticle (R=20 Å) in CO/O2 binary environment (T = 800K, P = 1000Pa)

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.

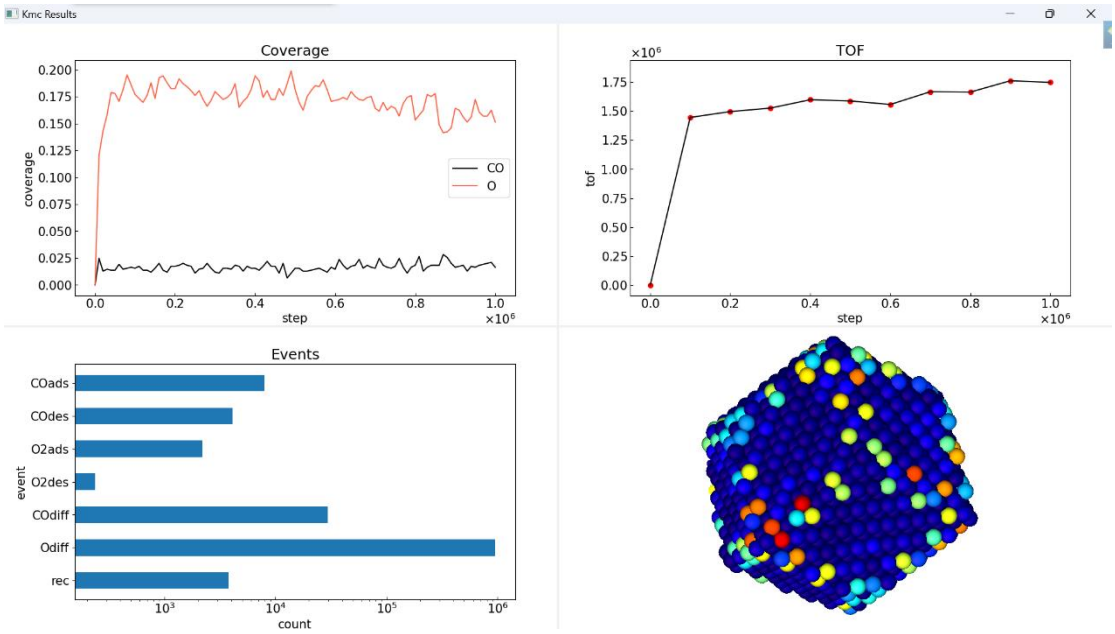


Fig 2. KMC Result analysis window