

1. Create a project:

New project → enter Redox on Pt → click the OK

2. Input the crystal structure of substrate Pt(111):

Module → Kinetix → select **Process Builder** → in the Description text box, enter Hexagonal ZGB model → Lattice Type: Hexagonal, Symmetry: p 6 m m, Length: 2.77 Å → Create and close the dialog

3. Specifying the processes:

In the Project Explorer, change the process filename KinetixProcesses.xkp to ZGBProcesses.xkp → Select the Species tab, enter CO and press the TAB key → Enter O in the next row and press the TAB key → Enter CO₂ in the next row and press the TAB key.

Select the Processes tab, the process of type: Adsorption → Click Add.

On the Process Details tab, Identifier: **COAds**, Description: CO adsorption → Specification type: Rates, Rate coefficient: 0.55.

On the Process Sites tab, uncheck the dissociative adsorption, and Adsorption Sites: select CO from the Adsorbate(s) list.

On the Processes tab, Process of type: Adsorption → Click the Add button.

On the Process Details tab, Identifier: **O₂Ads**, Description: O₂ adsorption → Specification type: Rates, Rate coefficient: 0.15.

On the Process Sites tab, check the Dissociative adsorption, Species: select O from the Adsorbate(s) dropdown lists.

On the Processes tab, process of type: Associative → Click Add button.

On the Process Details tab, Identifier: **CO₂form**, Description: CO₂ formation → Specification type: Immediate

On the Process Sites tab, Species: CO and O.

On the Processes tab, Process of type: Diffusion → Click the Add button.

On the Process Details tab, Identifier: **ODiff**, Description: O diffusion → Specification type: Rates, Rate coefficient: 15.

On the Process Sites tab, Species: select O from the Adsorbate(s) dropdown lists.

On the Processes tab, Process of type: Diffusion → Click the Add button.

On the Process Details tab, Identifier: **CODiff**, Description: CO diffusion → Specification type: Rates, Rate coefficient: 25.

On the Process Sites tab, Species: select CO from the Adsorbate(s) dropdown lists.

On the Processes tab, Process of type: Desorption → Click the Add button.

On the Process Details tab, Identifier: **CO₂Des**, Description: CO₂ desorption → Specification type: Rates, Rate coefficient: 5.

On the Process Sites tab, uncheck Associative desorption. Species: select CO₂ from the Adsorbate(s) dropdown lists.

On the Processes tab, Process of type: Desorption → Click the Add button.

On the Process Details tab, Identifier: **CODes**, Description: CO desorption → Specification type: Rates, Rate coefficient: 0.001.

On the Process Sites tab, uncheck Associative desorption. Species: select CO from the Adsorbate(s) dropdown lists.

On the Processes tab, Process of type: Desorption→Click the Add button.

On the Process Details tab, Identifier: **O2Des**, Description: O2 desorption→ Specification type: Rates, Rate coefficient: 0.001.

On the Process Sites tab, check Associative desorption. Species: select O from the Adsorbate(s) dropdown lists.

On the Site View tab and click the arrow buttons for the Process index to scroll through the processes defined→Check that none of the processes are shown by red sites→Select File | Save Project from the menu bar.

4. Creating an initial configuration:

Module→Kinetix→ Configuration Builder→Change the Configuration size to 64 × 64→ Type of configuration: Constant→In the Species to fill section, select V from the Adsorption sites dropdown list→Click Create and close the dialog→Rename the configuration document to ZGB.xkc→Select File | Save Project.

5. Running a Kinetix simulation:

Modules→Kinetix→Calculation→Ensure that ZGB.xkc is the active document→ On Setup tab, choose ZGBProcesses.xkp from the Processes dropdown list. Task: Constant conditions→ Close the Kinetix Constant Conditions dialog→ Click the Run button and close the dialog.

6. Analyzing the results of a Kinetix simulation:

In the Project Explorer, open ZGB.kout→ Modules→Kinetix→Analysis

Select Concentrations→check the checkboxes for the CO and O Species→Click the View button.

Select Rates→uncheck the checkboxes for the CODiff and ODiff→ Click the View button.

Open ZGBTraj.xkc→Click the Play button→Show animation of the trajectory→Stop.

Right-click in ZGBTraj.xkc→Select Display Style→On Options tab, Background color: white→On the Style tab, the Radius scale and the Vacancy scale:1.4→Close the dialog.

Right-click in ZGBTraj.xkc→Select Properties →Change the Color of one of the species and close the dialog→ File | Save Project→Window | Close All.