A Tutorial on

CATKINAS

A Catalytic microKinetic Analysis Software

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Why use CATKINAS?

- **Simple, but powerful:**
- 1. Generalized framework, simple inputs, easy to use
- 2. Efficient handling of large reaction mechanisms
- 3. Multi-level efficient and stable solver for steady-state
- 4. Multi-functional analyzer for reaction mechanisms and paths
- 5. Multi-dimensional simulation for catalyst descriptor and reaction condition
- **Free for educational and academic purposes**

Getting Started

- **How to install?**

  Run in MATLAB (version ≥R2014a)

  No additional installation is required!

- **How to run?**

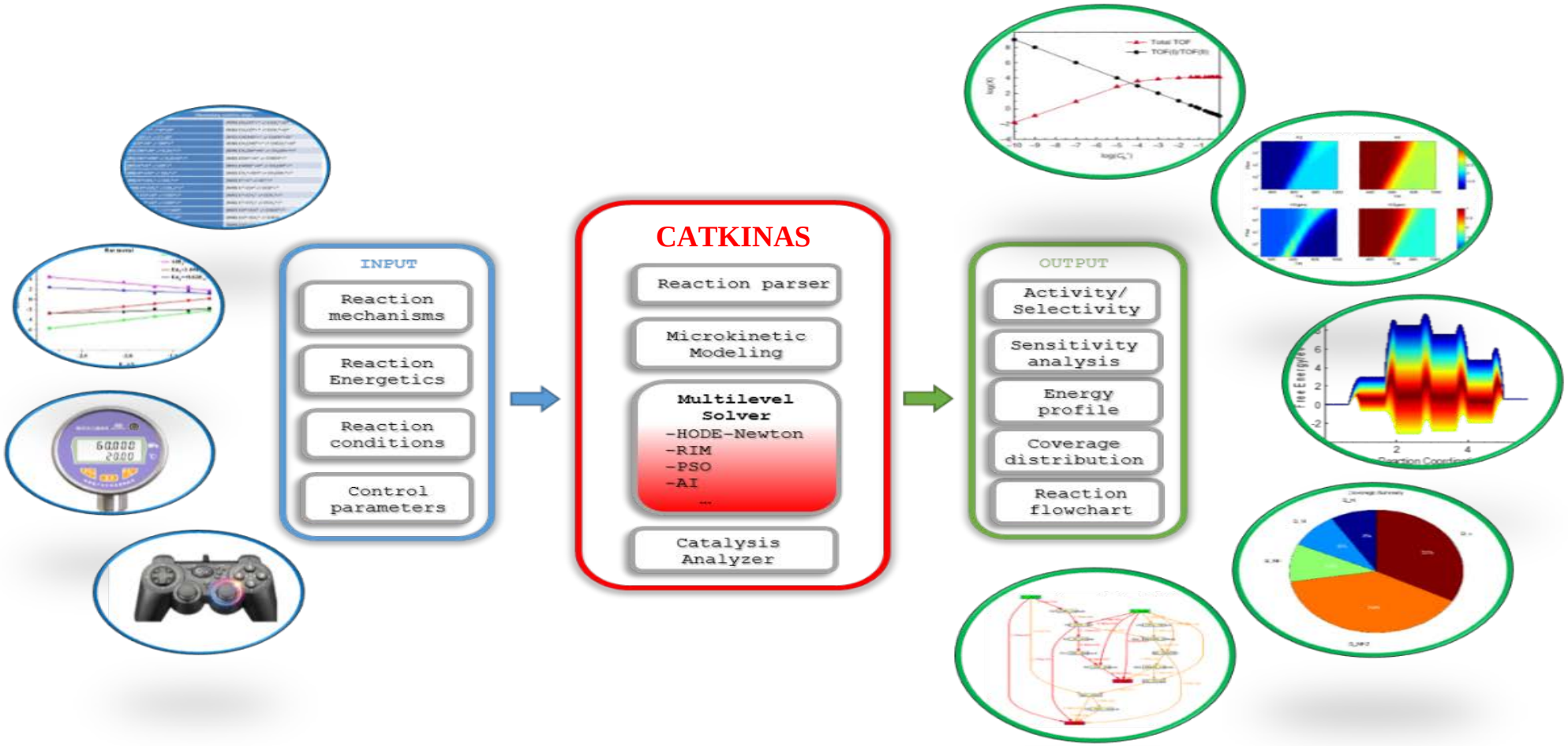
1. Start MATLAB, and at the prompt type: CATKINAS INPUT
2. Run in the background, save command "CATKINAS INPUT" to the file: Main.m

   and run the following command in the ***shell*** and ***cmd*** window, respectively:

   nohup MATLABPATH/matlab <Main.m> print-out &

   "MATLABPATH\matlab.exe" -nodesktop -nodisplay -nosplash -r "run('Main')"

The Framework of CATKINAS



Input/Output files

- CATKINAS basic input files:
  1. **CATKINAS.in**: parameters for simulation, solution and visualization
  2. **Thermodynamics.data** (optional): Thermodynamics data for energy correction
- CATKINAS basic output files:
  1. **log**: run result log in text format (log_parsum for parallel)
  2. **data.mat**: run result data in matrix format
  3. **fig**: visualization result for activity, coverage, reversibility, degree of rate control, energy profile, flow chart, etc.

程序手册

ReadMe.m.png (2471×5487像素, 685KB) - 2345看图王 - 第17/18张 100%

```
%  run with the command: CATLAB('INCAR'), CATLAB INCAR or Main
%
%% Input
%  INCAR is the input file which contains the reaction mechanisms and reaction conditions
%  simple matl                    table in INCAR file
%  '%' and '!'                    for seperation
%  From the reaction mechanism equations to the kinetic equations
%  examples :
%  {xx}: for note                 Energy input: [  Ea     G0    ]/[Ea(scaling);G0(scaling)]/[ Ea(BEP)   G0(scaling)]
%  {01}: H2 + 2#1 <-> 2H#1                      [  0.27  -0.20 ]/[ A1  B     ; a1  b     ]/[ A1  B     a1  b      ]
%  {02}: O2 + 2O#2 <-> 2O#2                     [  0.85   0.47 ]/[ for one Energy mode   ]/[ for one Energy mode  ]
%  {03}: H#1 + O#2 <-> #1 + OH#2                [  1.18   1.09 ]/[ A1  A2  B ; a1  a2  b ]/[ A1  B     a1  a2  b  ]
%  {04}: H#1 + OH#2 <-> #1 + #2 + H2O           [  1.18   1.09 ]/[ for two Energies mode ]/[ for two Energies mode]
%
%  #i for site i, e.g., #1 for site 1
%  forward and reverse reaction are separated by <-> ,
%  and use it as an identifier for the reaction mechanism equations
%  H2, O2, H2O for gas species
%  H#1, O#2, OH#2 for adsorbed species
%  Species(p) : relative pressure item of Species in rate equation
%  Species(c) : relative concentration item of Species in rate equation
%  format : variable = value; Or matlab command;
%
%  Istart : start from a previous run with new parameters setting or not : 1/0
%  npar : process number for parallel computing
%  runid : assign to the runid-th run : 1... , the last unfinished
%  Ndigits : digits for calculation in modified Newton Methods
%  TryMode : try modified newton Method in Mupad/Matlab: 0/1
%  MaxTime : maximum time for each newton try : s
%  MaxOdeTime : maximum time for each ode simulation try : s
%  TimeMode : auto increase the MaxTime for each PSO generation iteration or not : 1/0
%  SaveMode : save all the data in double or sym : 0/1
%  SaveFreq : save frequency for every N sample runs : 1
%  SkipMode : never skip the solution found by modified Newton Methods, or skip if it contains any/all zeros : 0/1/2
%  CheckMode : check the reaction thermodynamics, none/first/always : 0/1/2
%  TryOrderList : try order list of methods to get the initial guesses for modified Newton Method :
%           initial state(and neighbor state if available)/hybrid Newtomn and time-integation procedure(alternately)/
%           particle swarm optimization/reaction boundary condition/numeric::solve method : Init/ODE(2)/PSO/Boundary/solve
```

反应机理

反应能垒/焓变

书写规则说明

鸟瞰图 100%

程序手册

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```
%  X_Species_EQUI : deal with Reaction i in equilibrium to solve X_Species, X: Q/Qi
%
%  Energy input ways :
%        1. provide matlab function for calculating Ea/G0 by setting fun2GetGE = @funName
%        2. provide Ea/G0 beside reaction mechanism [Ea, G0]/[Ea(scaling) G0(scaling)]/[Ea(BEP) G0(scaling)]
%        3. provide Ea/G0 directly by setting Ea = [Ea1, Ea2...]/[Ea(scaling)'...]/[Ea(BEP)'...], G0 = ...
%  CalMode : calculate mode : 0 for single, >= 1 for curve, >= 2 for map
%  E1/E2 : energy (range) for descriptor
%  Available ranges : E(1/2)/T/P/C/Vgt/Vlt : energy(1/2)/temperature/pressure/concentration/gas/liquid volume flow rate
%                     range for descriptor, which are labeled 0/1/2/3/4/5, respectively
%  fun2E1/fun2E2 : A provided matlab function for calculating new E1 based on origin E1(for coverage effect etc.) :
%                  fun2E1 = @funName,i.e. E1 = funName(E1), or fun2E1 = @(E1) E1 + 0.2*Q1_I directly
%  when CalMode >= 1, curve: E1 : 1.0; T  : 1.1; P  : 1.2; C  : 1.3; Vgt: 1.4; Vlt: 1.5
%  when CalMode >= 2, map:   E1, E2 : 2.00; E1, T  : 2.01; E1, P  : 2.02; E1, C  : 2.03
%             E1, Vgt: 2.04; E1, Vlt: 2.05; T , P  : 2.12; T , C  : 2.13; T , Vgt: 2.14; T , Vlt: 2.15
%             P , C  : 2.23; P , Vgt: 2.24; P , Vlt: 2.25; C , Vgt: 2.34; C , Vlt: 2.35; Vgt,Vlt: 2.45
%  fun2GetGE : A provided matlab function for calculating Ea and G0 : fun2GetGE = @funName,i.e. [Ea, G0] = funName(var1,var2),
%             where [Ea, G0] = funName() for single, [Ea, G0] = funName(E1) for curve and [Ea, G0] = funName(E1, E2) for map;
%  Ea : energy barriers of each reaction for single,                                  eaction) and map(3/2*Nreaction);
%  G0 : Gibbs free energy of each reaction for single                                 ction) and map(3*Nreaction);
%  BEPMode : barrier input mode in scaling/BEP relationship, i.e. Ea = sum(alpha1 E1) + beta or alpha*G0 + beta : 1/0
%
%  ThermoMode : thermodynamics correction mode for reactant/product species with
%               none/dH/dH-TdS/dH-TdS+ZPE/-TdS/-TdS+ZPE/ZPE/dH+ZPE : 0/1/2/3/4/5/6/7
%  BarrierMode : barrier correction mode for adsorption/desorption reaction by none/
%                thermodynamics(TD)/transition-state theory(TST)/collision theory(CT) : -2/-1/0~1/2
%  ConsMode: mode for barrier constained, i.e. larger than none/0/E0/G0/(0,E0)/(0,G0)/(E0,G0)/All : 0/1/2/3/4/5/6/7
%  As : areas of the active site (for collision theory(CT)) : Angstrom^2;
%  Mr_Species : relative molecular mass for CT calculation, the value shoud be set
%               when species with a nonstandard chemical formula, or set the value to be -2/-1/0~1
%               to shift the species adsorption/desorption to none/TD/TST procedure
%  Thermo_Species : thermodynamics parameters for the Species, which is not in the database or overwrite it
%  Thermo_Species = [dGc]; n = 1; dGc : free energy correction for species
%                 = [G, H0, ZPE]; 1 < n <= 3; G = H0 + CpT - TdS; dGc = G - H0;
%                 = [H, H0, CpT, TdS, ZPE, Ef]; 3 < n <= 6; Ef : formation energy
%                 = [A, B, C, D, E, F, G, H, freqi, Ef]; n > 7; A-H : shomate equation parameters,
%                                                       freqi : frequency (cm^-1) for calclating ZPE
%
%  % Define default Thermodynamics data in file Thermodynamics_data
```

能垒处理、热力学校正

能量输入

程序手册

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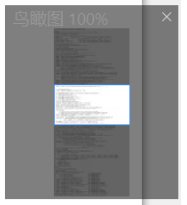
```
%  SimMode  : simplify the reaction energy profile and flow diagram with and without reaction sites : 1/0
%  SimValue : cut off value of reaction rate to simplify the reaction energy profile and flow diagram : 0.05
%  CompMode : compare the reaction energy profile and flow diagram in same/self ranges : 1/0
%
%  Q0 : initial coverage state
%  T  : temperature of the reaction
%  CalcDRC : calculate the degree of rate control or not : 1/0
%
%  set the reaction condition or freeze all the reactant and product pressure/concentration
%  Ns : number of active site : mol;
%  Ps : total relative pressure of gas : bar
%  Ng : total number of the gas molecular : mol
%  Vgt: rate of gas volume flow : m^3/h
%  Cs : total relative concentration of liquid : mol/L
%  Nl : total number of the liquid molecular : mol
%  Vlt: rate of liquid volume flow : m^3/h
%  P_Species : relative pressure of the Species
%  C_Species : relative concentration of the Species
%  Qi_Species : relative coverage of the Species at site i, v for vacancy
%  Q_Species : relative coverage of the Species for only one site case (#)
%  X_Species_INIT : the initial Species parameters X: P C Q/Qi
%  X_Species_FROZ : freeze the Species parameters X: P C
%  X_Species_RATE : sampling rate among pressures/concentrations for the Species parameters X: P C
%  X_Species_EQUI : deal with Reaction i in equilibrium to solve X_Species, X: Q/Qi
%
%  Energy input ways :
%        1. provide matlab function for calculating Ea/G0 by setting fun2GetGE = @funName
%        2. provide Ea/G0 beside reaction mechanism [Ea, G0]/[Ea(scaling) G0(scaling)]/[Ea(BEP)
%        3. provide Ea/G0 directly by setting Ea = [Ea1, Ea2...]/[Ea(scaling)'...]/[Ea(BEP)'...]
%  CalMode : calculate mode : 0 for single, >= 1 for curve, >= 2 for map
%  E1/E2 : energy (range) for descriptor
%  Available ranges : E(1/2)/T/P/C/Vgt/Vlt : energy(1/2)/temperature/pressure/concentration/gas/liquid volume flow rate
%                     range for descriptor, which are labeled 0/1/2/3/4/5, respectively
%  fun2E1/fun2E2 : A provided matlab function for calculating new E1 based on origin E1(for coverage effect etc.) :
%                  fun2E1 = @funName,i.e. E1 = funName(E1), or fun2E1 = @(E1) E1 + 0.2*Q1_I directly
%  when CalMode >= 1, curve: E1 : 1.0; T  : 1.1; P  : 1.2; C  : 1.3; Vgt: 1.4; Vlt: 1.5
%  when CalMode >= 2, map:   E1, E2 : 2.00; E1, T  : 2.01; E1, P  : 2.02; E1, C  : 2.03
%             E1, Vgt: 2.04; E1, Vlt: 2.05; T , P  : 2.12; T , C  : 2.13; T , Vgt: 2.14; T , Vlt: 2.15
%             P , C  : 2.23; P , Vgt: 2.24; P , Vlt: 2.25; C , Vgt: 2.34; C , Vlt: 2.35; Vgt,Vlt: 2.45
```

反应条件

模拟类型

能量、温度、压力、浓度、空速、流速及其组合



程序手册

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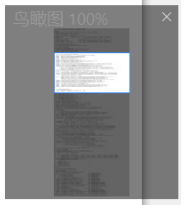
```
%
%  Istart : start from a previous run with new parameters setting or not : 1/0
%  npar : process number for parallel computing
%  runid : assign to the runid-th run : 1... , the last unfinished one for default
%  Ndigits : digits for calculation in modified Newton Methods
%  TryMode : try modified newton Method in Mupad/Matlab: 0/1
%  MaxTime : maximum time for each newton try : s
%  MaxOdeTime : maximum time for each ode simulation try : s
%  TimeMode : auto increase the MaxTime for each PSO generation iteration or not : 1/0
%  SaveMode : save all the data in double or sym : 0/1
%  SaveFreq : save frequency for every N sample runs : 1
%  SkipMode : never skip the solution found by modified Newton Methods, or skip if it contains any/all zeros : 0/1/2
%  CheckMode : check the reaction thermodynamics, none/first/always : 0/1/2
%  TryOrderList : try order list of methods to get the initial guesses for modified Newton Method :
%           initial state(and neighbor state if available)/hybrid Newtomn and time-integation procedure(alternately)/
%           particle swarm optimization/reaction boundary condition/numeric::solve method : Init/ODE(2)/PSO/Boundary/solve
%           TryOrderList = {'Init','ODE','ODE2','PSO','Boundary','solve'};
%  tspan : time span for ode simulation (s) : [0 1]
%  PlotType : plot the reaction curve/map, energy profile, flow diagram and ode simulation,
%             none/[curve/map]/profile/diagram/ode simulation/all/[1 ... 4] : 0/1/2/3/4/5/[specific]
%  PlotMode : plot the reaction energy profile, flow diagram and ode simulation, none/first/always/[1 ... n] : 0/1/inf/[specific]
%  ProfMode : plot the reaction energy profile in types of reaction total energy, standard free Gibbs energy, free Gibbs energy,
%             steady free Gibbs energy or all, 0/1/2/3/4
%  PlotList : assigned reaction results to plot : The reaction Rate/Select                    /erage/Apparent barrier/
%             Degree Rate Control of Barrier/Intermediate/[Pressure/Concen                    l/E2] :
%             Ri/Si_j/Zi/Yi/Xi_j/Ii_j/PCi_j/Gi_j, i/j are assigned index/T                    anations, e.g.
%             PlotList = {'R1+1/2*2-3','S1+2_3+4','Z-2-0.3*1+5','Y1+2+3','E3','X-2-3*1+5_1+2*2-3','I5_2','PC1_3',,'G1_3'};
%  PathOrder : assign reaction path orders list for energy profiles: PathOrder = {[1 2 3],[1 4]}
%  PathCoord : assign reaction path coordinations list for energy profiles: PathCoord = {[1 2 3],[1 3]}
%  PathScale : assign reaction path scales list for energy profiles: PathScale = {[1 2 1/2],[1 -1]}
%  FigMode   : save the output figures format as .fig/.png/both : 1/2/3
%  SimMode   : simplify the reaction energy profile and flow diagram with and without reaction sites : 1/0
%  SimValue : cut off value of reaction rate to simplify the reaction energy profile and flow diagram : 0.05
%  CompMode : compare the reaction energy profile and flow diagram in same/self ranges : 1/0
%
%  Q0 : initial coverage state
%  T  : temperature of the reaction
%  CalcDRC : calculate the degree of rate control or not : 1/0
%
```

动力学求解

数据可视化

控制参数



程序手册

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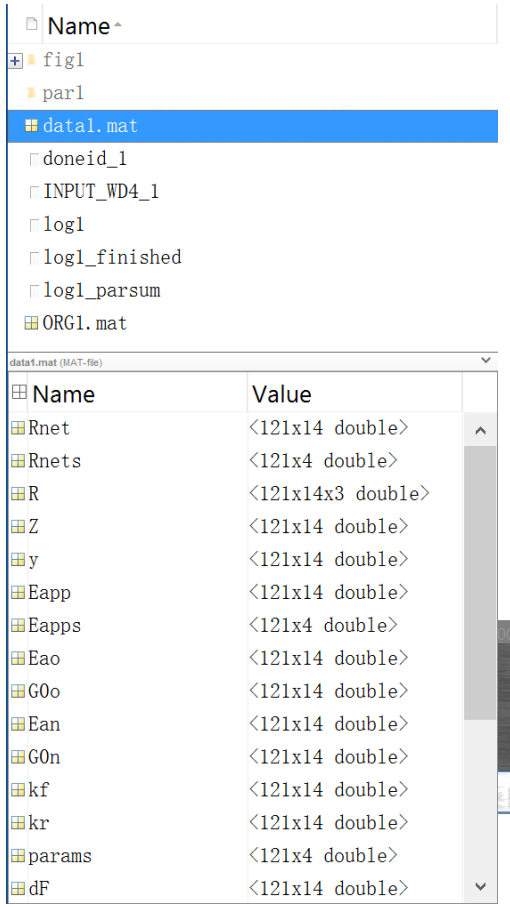
```
%       TR = [1000.00, 2500.00]; AH = [ 18.363083,  12.257357, -2.859786,  0.268258,   1.977990,  -1.147458, 156.288133, 0.000000];
%       TR = [2500.00, 6000.00]; AH = [ 43.413560,  -4.293079,  1.272428, -0.096876, -20.533862, -38.515158, 162.081354, 0.000000];
%  Or set Thermodynamics_data cell in file Thermodynamics_data.mat,
%  such as Thermodynamics_data{1} with fields of
%        ChemForm: 'H2'
%     form_energy: [ -0.272839]
%     frequencies: 4401
%     temperature: [3x2 double]
%      parameters: [3x8 double]
%  All the input energy in eV unit
%
```

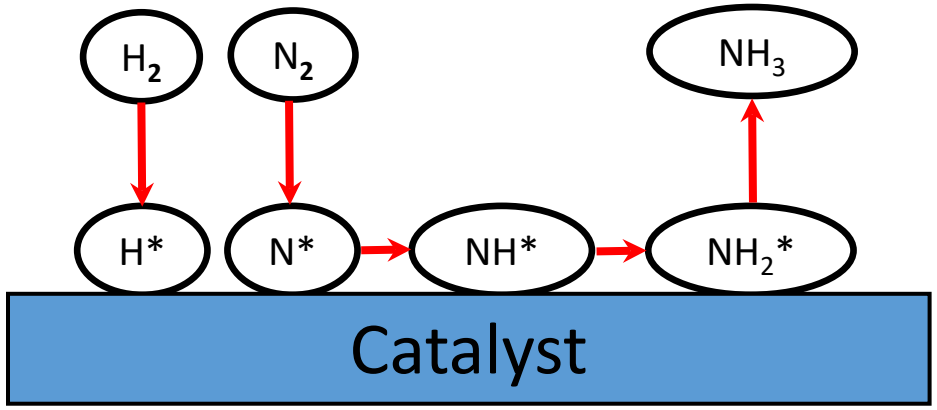
输出文件和数据

```
%% Output
%  all results are in result_INCAR directory
%  logi : run log file
%  datai.mat : calculation output results file
%  you can load the data by matlab command: load('datai.mat')
%  where  R : the reaction forward/reverse/net rate,                  size : Nsample*Nreaction*3
%      Rnet : the reaction net rate,                                  size : Nsample*Nreaction
%         Z : the reaction reversibility,                             size : Nsample*Nreaction
%         y : the coverage of species,                                size : Nsample*Nspecies
%        dF : the log10(residue) of steady-state equation,            size : Nsample*Nspecies
%      Eapp : the apparent reaction barrier,                          size : Nsample*Nreaction
%   Eao/Ean : the original/corrected reaction barrier,                size : Nsample*Nreaction
%   G0o/G0n : the original/corrected reaction Gibbs energy,           size : Nsample*Nreaction
%     kf/kr : the reaction forward/reverse rate constant,             size : Nsample*Nreaction
%     DRC_X : the degree of rate control of barrier,                  size : Nsample*Nbarrier*Nreaction
%     DRC_I : the degree of rate control of intermediate,             size : Nsample*Nsurspecies*Nreaction
%    DRC_PC : the degree of rate control of pressure/concentration,   size : Nsample*Nglspecies*Nreaction
%     DRC_G : the degree of rate control of descriptor E1/E2,         size : Nsample*NEdescriptors*Nreaction
%  Base on reactants/products :
%     Rnets : the reaction net rate,                                  size : Nsample*Nglspecies
%     Eapps : the apparent reaction barrier,                          size : Nsample*Nglspecies
%    DRC_Xs : the degree of rate control of barrier,                  size : Nsample*Nbarrier*Nglspecies
%    DRC_Is : the degree of rate control of intermediate,             size : Nsample*Nsurspecies*Nglspecies
%   DRC_PCs : the degree of rate control of pressure/concentration,   size : Nsample*Nglspecies*Nglspecies
%    DRC_Gs : the degree of rate control of descriptor E1/E2,         size : Nsample*NEdescriptors*Nglspecies
%  pari : parallel computing folder
%  figi : figure folder for calculating reaction curve/map, energy profile, flow diagram and ode simulation
```

17/18



Example: Ammonia synthesis



Requirements

- 1. Reaction mechanism
- 2. Reaction energy
- 3. Reaction condition
- 4. Control parameter (Optional)

Reaction mechanism **Reaction Energy**

```
%(x): for note          Energy input: [  Ea    |  H0    ]
  (1): H2 + 2#    <-> 2H#             [ 1.209   -0.757 ]
  (2): N2 + 2#    <-> 2N#             [ 0.658   -1.175 ]
  (3): N# + H#    <-> NH# + #         [ 1.429   -0.083 ]
  (4): NH# + H#   <-> NH2# + #        [ 1.592   -0.158 ]
  (5): NH2# + H# <-> NH3 + 2#         [ 1.986    1.435 ]
CalcDRC = 1;          % calculate the degree of rate control
T = 673;              % reaction temperature
P_H2_FROZ = 75;       % H2 pressure
P_N2_FROZ = 25;       % N2 pressure
P_NH3_FROZ = 1;       % NH3 pressure,  1% coversion
Q_v_INIT = 1;         % initial coverage of free site
ThermoMode = 4;       % only include entropy correction
BarrierMode = 1;      % deal the adsorption with collision theory
Mr_NH3 = -2;          % the barrier of the NH3 desorption is used by given
npar = 8;             % the process number for parallel computing
```

Reaction condition

例子：光解水析氧反应

输入文件

```
%% 反应机理                                          反应能垒和反应焓变
%{xx}: for note                          Energy input: [Ea(scaling);G0(scaling)]/[ Ea(BEP)   G0(scaling)]
{01}: H2O(c) + #1 <-> OH_minus#1 + proton(c)          [ 1.00  0.00;   0.00   0.11  ]
{02}: OH_minus#1 + hole(c) <-> OH_rad#1               [ 0.00  0.25;   0.00  -0.19  ]
{03}: OH_rad#1 <-> O_minus#1 + proton(c)              [ 0.00  0.41;   0.00  -0.54  ]
{04}: O_minus#1 + O_minus#1 <-> O2_2minus#1 + #1      [ 0.00  0.24;   0.00  -1.35  ]
{05}: O2_2minus#1 + hole(c) <-> O2_minus#1            [ 0.00  0.25;   0.00  -1.55  ]
{06}: O2_minus#1 + hole(c) <-> O2(p) + #1             [ 0.00  0.25;   0.00  -1.13  ]
{07}: #2 + hole(c) <-> Obr_minus#2                    [ 0.00  0.25;   0.00   0.05  ]
{08}: Obr_minus#2 + OH_rad#1 <-> ObrOH_minus#2 + #1   [ 0.00  0.32;   0.00  -1.62  ]
{09}: ObrOH_minus#2 + hole(c) <-> ObrOH#2             [ 0.00  0.25;   0.00  -1.22  ]
{10}: ObrOH#2 <-> ObrO_minus#2 + proton(c)            [ 0.00  0.23;   0.00  -0.18  ]
{11}: ObrO_minus#2 + hole(c) <-> O2(p) + Ovac#2       [ 0.00  0.25;   0.00  -1.27  ]
{12}: H2O(c) + Ovac#2 <-> H2O#2                       [ 0.00  0.00;   0.00  -0.91  ]
{13}: H2O#2 <-> OH_minus#2 + proton(c)                [ 0.00  0.32;   0.00  -0.11  ]
{14}: OH_minus#2 <-> #2 + proton(c)                   [ 0.00  0.37;   0.00  -0.25  ]
```

```
%% 反应条件
T = 300;
Q0 = [1 1];
C_H2O_INIT = 0;
C_hole_INIT = 1E-9;
C_proton_INIT = 0;
C_H2O_FROZ = 1;
C_hole_FROZ = 1E-9;
C_proton_FROZ = 1e-7;
P_O2_FROZ = 1e-7;
Q1_v_INIT = 1;
Q2_v_INIT = 1;
```

```
%% 控制参数
npar = 32;
Ndigits = 1000;
MaxTime = 30;
CalcDRC = 0;
CheckMode = 1;
ThermoMode = 0;
BarrierMode = -2;
ConsMode = 5;
E1 = [0:0.15:1.5];
C = 10.^[-10:1:0];
PlotMode = [1:5:121];
PlotType = 5;
```

输出文件

G:\CATLAB\oxygen evolution reaction\result_WD4\log1

```
Reaction : 11 : hole(liq) + #2 <-> Obr_minus#2
                + R7
Q2_Obr_minus = C_hole*Q2_v*z7*Keq(7)
Reaction : 12 : H2O(liq) + 4 hole(liq) + #2 <-> O2(gas) + 2 proton(liq) + Ovac#2
                + R1 + R2 + R7 + R8 + R9 + R10 + R11
Q2_Ovac = (C_H2O*C_hole^4*Q2_v*z1*z2*z7*z8*z9*z10*z11*Keq(9)*Keq(10)*Keq(11))/(C_proton^2*P_O2)
Reversibility relations Summary:
zt(1) = z1^2*z2^2*z3^2*z4*z5*z6 = (C_proton^4*P_O2)/(C_H2O^2*C_hole^4*Keq(1)^2*Keq(2)^2*Keq(3)^2*Keq(4)*Keq(5)*Keq(6))
1 = (z7*z8*z9*z10*z11*z12*z13*z14)/(z1*z2*z3^2*z4*z5*z6) = (Keq(1)*Keq(2)*Keq(3)^2*Keq(4)*Keq(5)*Keq(6))/(Keq(7)*Keq(8)*Keq(9)*Keq(10)*Keq(11)*Keq(12)*Keq(13)*Keq(14))
Coverage relations Summary:
Q1_O2_2minus = (C_H2O^2*C_hole^2*Q1_v*z1^2*z2^2*z3^2*z4*Keq(1)^2*Keq(2)^2*Keq(3)^2*Keq(4))/C_proton^4
Q1_O2_minus = (C_H2O^2*C_hole^3*Q1_v*z1^2*z2^2*z3^2*z4*z5*Keq(1)^2*Keq(2)^2*Keq(3)^2*Keq(4)*Keq(5))/C_proton^4
Q1_OH_minus = (C_H2O*Q1_v*z1*Keq(1))/C_proton
Q1_OH_rad = (C_H2O*C_hole*Q1_v*z1*z2*Keq(1)*Keq(2))/C_proton
Q1_O_minus = (C_H2O*C_hole*Q1_v*z1*z2*z3*Keq(1)*Keq(2)*Keq(3))/C_proton^2
Q2_H2O = (C_H2O^2*C_hole^4*Q2_v*z1*z2*z7*z8*z9*z10*z11*z12*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9)*Keq(10)*Keq(11)*Keq(12))/(C_proton^2*P_O2)
Q2_OH_minus = (C_H2O^2*C_hole^4*Q2_v*z1*z2*z7*z8*z9*z10*z11*z12*z13*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9)*Keq(10)*Keq(11)*Keq(12)*Keq(13))/(C_proton^3*P_O2)
Q2_ObrOH = (C_H2O*C_hole^3*Q2_v*z1*z2*z7*z8*z9*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9))/C_proton
Q2_ObrOH_minus = (C_H2O*C_hole^2*Q2_v*z1*z2*z7*z8*Keq(1)*Keq(2)*Keq(7)*Keq(8))/C_proton
Q2_ObrO_minus = (C_H2O*C_hole^3*Q2_v*z1*z2*z7*z8*z9*z10*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9)*Keq(10))/C_proton^2
Q2_Obr_minus = C_hole*Q2_v*z7*Keq(7)
Q2_Ovac = (C_H2O*C_hole^4*Q2_v*z1*z2*z7*z8*z9*z10*z11*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9)*Keq(10)*Keq(11))/(C_proton^2*P_O2)
Coverage expressions:
Q1_v = 1/((C_H2O*z1*Keq(1))/C_proton + (C_H2O*C_hole*z1*z2*Keq(1)*Keq(2))/C_proton + (C_H2O*C_hole*z1*z2*z3*Keq(1)*Keq(2)*Keq(3))/C_proton^2 + (C_H2O^2*C_hole^2*z1^2*z2^2*z3^2*z4*Keq(1)^2*Keq(2)^2*Keq(3)^2
Q2_v = 1/(C_hole*z7*Keq(7) + (C_H2O*C_hole^2*z1*z2*z7*z8*Keq(1)*Keq(2)*Keq(7)*Keq(8))/C_proton + (C_H2O*C_hole^3*z1*z2*z7*z8*z9*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9))/C_proton + (C_H2O*C_hole^3*z1*z2^2*z7*z8*z9
Reversibility expressions:
z1 = (C_proton*Q1_OH_minus)/(C_H2O*Q1_v*Keq(1))
z2 = Q1_OH_rad/(C_hole*Q1_OH_minus*Keq(2))
z3 = (C_proton*Q1_O_minus)/(Q1_OH_rad*Keq(3))
z4 = (Q1_v*Q1_O2_2minus)/(Q1_O_minus^2*Keq(4))
z5 = Q1_O2_minus/(C_hole*Q1_O2_2minus*Keq(5))
```

覆盖度公式

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可逆度公式

速率表达式

```
Reversibility expressions:
z1 = (C_proton*Q1_OH_minus)/(C_H2O*Q1_v*Keq(1))
z2 = Q1_OH_rad/(C_hole*Q1_OH_minus*Keq(2))
z3 = (C_proton*Q1_O_minus)/(Q1_OH_rad*Keq(3))
z4 = (Q1_v*Q1_O2_2minus)/(Q1_O_minus^2*Keq(4))
z5 = Q1_O2_minus/(C_hole*Q1_O2_2minus*Keq(5))
z6 = (P_O2*Q1_v)/(C_hole*Q1_O2_minus*Keq(6))
z7 = Q2_Obr_minus/(C_hole*Q2_v*Keq(7))
z8 = (Q1_v*Q2_ObrOH_minus)/(Q1_OH_rad*Q2_Obr_minus*Keq(8))
z9 = Q2_ObrOH/(C_hole*Q2_ObrOH_minus*Keq(9))
z10 = (C_proton*Q2_ObrO_minus)/(Q2_ObrOH*Keq(10))
z11 = (P_O2*Q2_Ovac)/(C_hole*Q2_ObrO_minus*Keq(11))
z12 = Q2_H2O/(C_H2O*Q2_Ovac*Keq(12))
z13 = (C_proton*Q2_OH_minus)/(Q2_H2O*Keq(13))
z14 = (C_proton*Q2_v)/(Q2_OH_minus*Keq(14))
Reaction rates:
r(1) = -C_H2O*Q1_v*kf(1)*(z1 - 1)
r(2) = -(C_H2O*C_hole*Q1_v*z1*Keq(1)*kf(2)*(z2 - 1))/C_proton
r(3) = -(C_H2O*C_hole*Q1_v*z1*z2*Keq(1)*Keq(2)*kf(3)*(z3 - 1))/C_proton
r(4) = -(C_H2O^2*C_hole^2*Q1_v^2*z1^2*z2^2*z3^2*Keq(1)^2*Keq(2)^2*Keq(3)^2*kf(4)*(z4 - 1))/C_proton^4
r(5) = -(C_H2O^2*C_hole^3*Q1_v*z1^2*z2^2*z3^2*z4*Keq(1)^2*Keq(2)^2*Keq(3)^2*Keq(4)*kf(5)*(z5 - 1))/C_proton^4
r(6) = -(C_H2O^2*C_hole^4*Q1_v*z1^2*z2^2*z3^2*z4*z5*Keq(1)^2*Keq(2)^2*Keq(3)^2*Keq(4)*Keq(5)*kf(6)*(z6 - 1))/C_proton^4
r(7) = -C_hole*Q2_v*kf(7)*(z7 - 1)
r(8) = -(C_H2O*C_hole^2*Q1_v*Q2_v*z1*z2*z7*Keq(1)*Keq(2)*Keq(7)*kf(8)*(z8 - 1))/C_proton
r(9) = -(C_H2O*C_hole^3*Q2_v*z1*z2*z7*z8*Keq(1)*Keq(2)*Keq(7)*Keq(8)*kf(9)*(z9 - 1))/C_proton
r(10) = -(C_H2O*C_hole^3*Q2_v*z1*z2*z7*z8*z9*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9)*kf(10)*(z10 - 1))/C_proton
r(11) = -(C_H2O*C_hole^4*Q2_v*z1*z2*z7*z8*z9*z10*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9)*Keq(10)*kf(11)*(z11 - 1))/C_proton^2
r(12) = -(C_H2O^2*C_hole^4*Q2_v*z1*z2*z7*z8*z9*z10*z11*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9)*Keq(10)*Keq(11)*kf(12)*(z12 - 1))/(C_proton^2*P_O2)
r(13) = -(C_H2O^2*C_hole^4*Q2_v*z1*z2*z7*z8*z9*z10*z11*z12*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9)*Keq(10)*Keq(11)*Keq(12)*kf(13)*(z13 - 1))/(C_proton^2*P_O2)
r(14) = -(C_H2O^2*C_hole^4*Q2_v*z1*z2*z7*z8*z9*z10*z11*z12*z13*Keq(1)*Keq(2)*Keq(7)*Keq(8)*Keq(9)*Keq(10)*Keq(11)*Keq(12)*Keq(13)*kf(14)*(z14 - 1))/(C_proton^3*P_O2)
```

```
The rate equations of every reaction :
r(1) = C_H2O*Q1_v*kf(1) - C_proton*Q1_OH_minus*kr(1)
r(2) = C_hole*Q1_OH_minus*kf(2) - Q1_OH_rad*kr(2)
r(3) = Q1_OH_rad*kf(3) - C_proton*Q1_O_minus*kr(3)
r(4) = Q1_O_minus^2*kf(4) - Q1_v*Q1_O2_2minus*kr(4)
r(5) = C_hole*Q1_O2_2minus*kf(5) - Q1_O2_minus*kr(5)
r(6) = C_hole*Q1_O2_minus*kf(6) - P_O2*Q1_v*kr(6)
r(7) = C_hole*Q2_v*kf(7) - Q2_Obr_minus*kr(7)
r(8) = Q1_OH_rad*Q2_Obr_minus*kf(8) - Q1_v*Q2_ObrOH_minus*kr(8)
r(9) = C_hole*Q2_ObrOH_minus*kf(9) - Q2_ObrOH*kr(9)
r(10) = Q2_ObrOH*kf(10) - C_proton*Q2_ObrO_minus*kr(10)
r(11) = C_hole*Q2_ObrO_minus*kf(11) - P_O2*Q2_Ovac*kr(11)
r(12) = C_H2O*Q2_Ovac*kf(12) - Q2_H2O*kr(12)
r(13) = Q2_H2O*kf(13) - C_proton*Q2_OH_minus*kr(13)
r(14) = Q2_OH_minus*kf(14) - C_proton*Q2_v*kr(14)
```

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157 r(14) = -(C_H2O^2*C_hole^4*Q2_v*z1*z2*z7*z8*z9*z (2)*Keq(7)*Keq(8)*Keq(9)*Keq(10)*Keq(11)*Keq(12)*Keq(13)*kf(14)*(z14 - 1))/(C_proton^3*P_02)

158

159 Try to generate the kinetic rate equations in myl v ...

160

稳态方程

```
The equations based on rate of every reaction :
dQ1_O2_2minus/dt = r(4) - r(5)
dQ1_O2_minus/dt = r(5) - r(6)
dQ1_OH_minus/dt = r(1) - r(2)
dQ1_OH_rad/dt = r(2) - r(3) - r(8)
dQ1_O_minus/dt = r(3) - 2*r(4)
dQ1_v/dt = r(4) - r(1) + r(6) + r(8)
dQ2_H2O/dt = r(12) - r(13)
dQ2_OH_minus/dt = r(13) - r(14)
dQ2_ObrOH/dt = r(9) - r(10)
dQ2_ObrOH_minus/dt = r(8) - r(9)
dQ2_ObrO_minus/dt = r(10) - r(11)
dQ2_Obr_minus/dt = r(7) - r(8)
dQ2_Ovac/dt = r(11) - r(12)
dQ2_v/dt = r(14) - r(7)
dC_H2O/dt = -(Cs*(Ns*r(1) + Ns*r(12) + CO*NA*Vlt*(C_H2O - Co_H2O)))/Nl
dC_hole/dt = -(Cs*(Ns*r(2) + Ns*r(5) + Ns*r(6) + Ns*r(7) + Ns*r(9) + Ns*r(11) + CO*NA*Vlt*(C_hole - Co_hole)))/Nl
dC_proton/dt = (Cs*(Ns*r(1) + Ns*r(3) + Ns*r(10) + Ns*r(13) + Ns*r(14) - CO*NA*Vlt*(C_proton - Co_proton)))/Nl
dP_O2/dt = (Ps*(Ns*r(6) + Ns*r(11) - (PO*Vgt*(P_O2 - Po_O2))/(T*kB)))/Ng
```

181 The rate equations of every reaction :

```
r(1) = C_H2O*Q1_v*kf(1) - C_proton*Q1_OH_minus*kr(1)
r(2) = C_hole*Q1_OH_minus*kf(2) - Q1_OH_rad*kr(2)
r(3) = Q1_OH_rad*kf(3) - C_proton*Q1_O_minus*kr(3)
r(4) = Q1_O_minus^2*kf(4) - Q1_v*Q1_O2_2minus*kr(4)
r(5) = C_hole*Q1_O2_2minus*kf(5) - Q1_O2_minus*kr(5)
```

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运行进度

```
The maximum available cpu in this computer is only 8, reset npar = 8

Solve the reaction kinetics ...
Progress : [============================================================================================================]
Ratio    :  121/ 121; Percent : 100%; Used Time :      00:02:47; Left Time :      00:00:00

Plot the reaction result ...
Progress : [============================================================================================================]
Ratio    :   32/  32; Percent : 100%; Used Time :      00:00:30; Left Time :      00:00:00

The possible reaction pathways :
Total Rection(s):
Reaction :  1 : 2 H2O(liq) + 4 hole(liq) <-> O2(gas) + 4 proton(liq)
                + 2 R1 + 2 R2 + 2 R3 + R4 + R5 + R6
Reaction :  2 : 2 H2O(liq) + 4 hole(liq) <-> O2(gas) + 4 proton(liq)
                + R1 + R2 + R7 + R8 + R9 + R10 + R11 + R12 + R13 + R14

Plot the reaction energy profile ...
Progress : [============================================================================================================]
Ratio    :   11/  11; Percent : 100%; Used Time :      00:00:07; Left Time :      00:00:00

Plot the reaction flow diagram ...
Progress : [============================================================================================================]
Ratio    :   25/  25; Percent : 100%; Used Time :      00:00:19; Left Time :      00:00:00

Plot the ode simulation result ...
Progress : [============================================================================================================]
Ratio    :   25/  25; Percent : 100%; Used Time :      00:00:51; Left Time :      00:00:00

Elapsed time: 00:04:51.239
```

动力学求解

绘制活性、覆盖度、可逆度

简化反应路径

绘制反应势能图

绘制反应流程图

绘制反应演化图

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输入数据校验

能垒处理、热力学校正

```
Run the sample 1 now @ E1/eV: 0 and C/mol/L: 1e-10 ...
```

Type		Original			Corrected			Corrected			TS mode	
Reactions	Ea/for	Ea/rev	G0	Ea/for	Ea/rev	G0	k/for	k/rev	Keq	forward	reverse
{01}:H2O(c)+#1<->OH_minus#1+proton(c)	0.00	-0.11	0.11	0.11	0.00	0.11	8.87e+10	6.25e+12	1.42e-02	ORI	TST
{02}:OH_minus#1+hole(c)<->OH_rad#1	0.25	0.44	-0.19	0.25	0.44	-0.19	3.95e+08	2.54e+05	1.56e+03	ORI	TST
{03}:OH_rad#1<->O_minus#1+proton(c)	0.41	0.95	-0.54	0.41	0.95	-0.54	8.10e+05	6.87e-04	1.18e+09	ORI	TST
{04}:O_minus#1+O_minus#1<->O2_2minus#1+#1	0.24	1.59	-1.35	0.24	1.59	-1.35	5.81e+08	1.22e-14	4.78e+22	TST	TST
{05}:O2_2minus#1+hole(c)<->O2_minus#1	0.25	1.80	-1.55	0.25	1.80	-1.55	3.95e+08	3.61e-18	1.09e+26	ORI	TST
{06}:O2_minus#1+hole(c)<->O2(p)+#1	0.25	1.38	-1.13	0.25	1.38	-1.13	3.95e+08	4.10e-11	9.62e+18	ORI	TST
{07}:#2+hole(c)<->Obr_minus#2	0.25	0.20	0.05	0.25	0.20	0.05	3.95e+08	2.73e+09	1.45e-01	ORI	TST
{08}:Obr_minus#2+OH_rad#1<->ObrOH_minus#2+#1	0.32	1.94	-1.62	0.32	1.94	-1.62	2.63e+07	1.60e-20	1.64e+27	TST	TST
{09}:ObrOH_minus#2+hole(c)<->ObrOH#2	0.25	1.47	-1.22	0.25	1.47	-1.22	3.95e+08	1.26e-12	3.13e+20	ORI	TST
{10}:ObrOH#2<->Obr0_minus#2+proton(c)	0.23	0.41	-0.18	0.23	0.41	-0.18	8.55e+08	8.10e+05	1.06e+03	ORI	TST
{11}:Obr0_minus#2+hole(c)<->O2(p)+0vac#2	0.25	1.52	-1.27	0.25	1.52	-1.27	3.95e+08	1.82e-13	2.16e+21	ORI	TST
{12}:H2O(c)+0vac#2<->H2O#2	0.00	0.91	-0.91	0.00	0.91	-0.91	6.25e+12	3.23e-03	1.94e+15	ORI	TST
{13}:H2O#2<->OH_minus#2+proton(c)	0.32	0.43	-0.11	0.32	0.43	-0.11	2.63e+07	3.73e+05	7.05e+01	ORI	TST
{14}:OH_minus#2<->#2+proton(c)	0.37	0.62	-0.25	0.37	0.62	-0.25	3.80e+06	2.40e+02	1.58e+04	ORI	TST

```
Inner cycle(s):
dG = -0.32 eV :  - R1 - R2 - 2 R3 - R4 - R5 - R6 + R7 + R8 + R9 + R10 + R11 + R12 + R13 + R14
Total rection(s):
Reaction :  1 : 2 H2O(liq) + 4 hole(liq) <-> O2(gas) + 4 proton(liq)
dG = -5.27 eV :  + 2 R1 + 2 R2 + 2 R3 + R4 + R5 + R6

Try numeric::fsolve now ...
Elapsed time: 00:00:00.607. Converged, r                    ~= 10^-1014. Succeed!!
Extract individual solutions by numeric:
Q1_O2_2minus      =   2.1613554174e-01
Q1_O2_minus       =   2.1613554174e-01
Q1_OH_minus       =   5.6772106404e-01
```

反应机理、热力学恒算

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```
{11}:OBrO_minus#2+hole(c)<->O2(p)+Ovac#2          0.25    1.52    -1.27    0.25    1.52    -1.27    3.95e+08    1.82e-13    2.16e+21    ORI    TST
{12}:H2O(c)+Ovac#2<->H2O#2                        0.00    0.91    -0.91    0.00    0.91    -0.91    6.25e+12    3.23e-03    1.94e+15    ORI    TST
{13}:H2O#2<->OH_minus#2+proton(c)                 0.32    0.43    -0.11    0.32    0.43    -0.11    2.63e+07    3.73e+05    7.05e+01    ORI    TST
{14}:OH_minus#2<->#2+proton(c)                    0.37    0.62    -0.25    0.37    0.62    -0.25    3.80e+06    2.40e+02    1.58e+04    ORI    TST
Inner cycle(s):
dG = -0.32 eV :  - R1 - R2 - 2 R3 - R4 - R5 - R6 + R7 + R8 + R9 + R10 + R11 + R12 + R13 + R14
Total rection(s):
Reaction :  1 * 2 H2O(liq) + 4 hole(liq) <-> O2(gas) + 4 proton(liq)
dG = -5.27 eV  + R5 + R6

Try numeric::fsolve now ...
Elapsed time: 00:00:00.607. Converged, return with the residue |dy/dt| ~= 10^-1021, |dlog(y)/dt| ~= 10^-1014. Succeed!!
Extract individual solutions by numeric::fsolve
Q1_O2_2minus      =   2.1613554174e-01
Q1_O2_minus       =   2.1613554174e-01
Q1_OH_minus       =   5.6772106404e-01
Q1_OH_rad         =   2.1068556868e-08
Q1_O_minus        =   3.8314828689e-06
Q1_v              =   3.9999224308e-06
Q2_H2O            =   3.1351918608e-19
Q2_OH_minus       =   6.3123318995e-12
Q2_OBrOH          =   2.8594856082e-20
Q2_OBrOH_minus    =   2.0310744146e-10
Q2_OBrO_minus     =   2.0310744146e-10
Q2_OBr_minus      =   1.4455660365e-11
Q2_Ovac           =   1.2820811545e-24
Q2_v              =   9.9999999957e-01
Elapsed time: 00:00:00.128. Converged, return with the residue |dy/dt| ~= 10^-1028, |dlog(y)/dt| ~= 10^-1018. Succeed!!
Extract individual solutions by numeric::fsolve
 No.                Rforward                Rreverse                  Rnet           Reversibility    Reactions                                                    Ea          G0        Eapp          kf
```

稳态覆盖度

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稳态速率、可逆度

```
Q2_0vac              =    1.2820
Q2_v                 =    9.9999
Elapsed time: 00:00:00.128. Converged, return with the residue |dy/dt|  10^-1028, |dlog(y)/dt| ~= 10^-1018. Succeed!!
Extract individual solutions by numeric::fsolve
```

No.	Rforward	Rreverse	Rnet	Reversibility	Reactions	Ea	G0	Eapp	kf
1 :	3.5488206107043097e+05	3.5488204401373595e+05	1.7056695000973014e-02	9.9999995193700419e-01	{01}:H2O(c)+#1<->OH_minus#1+proton(c)	0.11	0.11	0.25	8.87e+10
2 :	2.2401325002549349e-02	5.3446300015763367e-03	1.7056695000973014e-02	2.3858544085977501e-01	{02}:OH_minus#1+hole(c)<->OH_rad#1	0.25	-0.19	0.25	3.95e+08
3 :	1.7056694992958994e-02	2.6304902345782641e-16	1.7056694992958733e-02	1.5422039472852921e-14	{03}:OH_rad#1<->O_minus#1+proton(c)	0.41	-0.54	0.25	8.10e+05
4 :	8.5283474964793667e-03	1.0517999539519397e-20	8.5283474964793667e-03	1.2332986600113785e-18	{04}:O_minus#1+O_minus#1<->O2_2minus#1+#1	0.24	-1.35	0.25	5.81e+08
5 :	8.5283474964793667e-03	7.7990357346324256e-19	8.5283474964793667e-03	9.1448381270251805e-17	{05}:O2_2minus#1+hole(c)<->O2_minus#1	0.25	-1.55	0.25	3.95e+08
6 :	8.5283474964793667e-03	1.6407696965098282e-23	8.5283474964793667e-03	1.9239010807042787e-21	{06}:O2_minus#1+hole(c)<->O2(p)+#1	0.25	-1.13	0.25	3.95e+08
7 :	3.9458329824163557e-02	3.9458329816149273e-02	8.0142804183078196e-12	9.9999999979689258e-01	{07}:#2+hole(c)<->Obr_minus#2	0.25	0.05	0.21	3.95e+08
8 :	8.0142804183078196e-12	1.3037620858027414e-35	8.0142804183078196e-12	1.6267986865351352e-24	{08}:Obr_minus#2+OH_rad#1<->ObrOH_minus#2+#1	0.32	-1.62	0.21	2.63e+07
9 :	8.0142804183078196e-12	3.6087122795186601e-32	8.0142804183078196e-12	4.5028525221988976e-21	{09}:ObrOH_minus#2+hole(c)<->ObrOH#2	0.25	-1.22	0.21	3.95e+08
10 :	2.4457464930239748e-11	1.6443184511931928e-11	8.0142804183078196e-12	6.7231761586219074e-01	{10}:ObrOH#2<->ObrO_minus#2+proton(c)	0.23	-0.18	0.21	8.55e+08
11 :	8.0142804183078196e-12	2.3389330733540554e-44	8.0142804183078196e-12	2.9184567438032203e-33	{11}:ObrO_minus#2+hole(c)<->O2(p)+0vac#2	0.25	-1.27	0.21	3.95e+08
12 :	8.0142804193191755e-12	1.0113548926576328e-21	8.0142804183078196e-12	1.2619409850192749e-10	{12}:H2O(c)+0vac#2<->H2O#2	0.00	-0.91	0.21	6.25e+12
13 :	8.2500376889244972e-12	2.3575727061667662e-13	8.0142804183078196e-12	2.8576508315007555e-02	{13}:H2O#2<->OH_minus#2+proton(c)	0.32	-0.11	0.21	2.63e+07
14 :	2.4011515494393395e-05	2.4011507480112977e-05	8.0142804183078196e-12	9.9999966623179537e-01	{14}:OH_minus#2<->#2+proton(c)	0.37	-0.25	0.21	3.80e+06

```
Base on reactants/products :
```

No.	gas1	liq1	liq2	liq3
Rate :	8.5283475044936469e-03	-1.7056695008987294e-02	-3.4113390017974587e-02	3.4113390017974587e-02
Eapp :	0.25	0.25	0.25	0.25

```
Elapsed time: 00:00:02.604. Try numeric::fsolve finished ...

Calculate the degree of                                    (c))
Elapsed time: 00:00:00.124. Converged, return with the residue |dy/dt|  10^-1021, |dlog(y)/dt| ~= 10^-1014. Succeed!!
Extract individual solutions by numeric::fsolve
```

反应物和产物速率、表观能垒

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输出文件

G:\CATLAB\oxygen evolution reaction\result_WD4\log1_parsum

EDITOR VIEW

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FILE EDIT NAVIGATE BREAKPOINTS

```
134  0.00    0.00    -0.00   -0.00   -0.00   -0.00   0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    {10}:ObrOH#2<->Obr0_minus#2+proton(c)
135  0.00    0.00    -0.00   -0.00   -0.00   -0.00   0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    {11}:Obr0_minus#2+hole(c)<->02(p)+0vac#2
136  0.00    0.00    -0.     能垒敏感度      ).00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    {12}:H20(c)+0vac#2<->H20#2
137  0.00    0.00    -0.             ).00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    {13}:H20#2<->OH_minus#2+proton(c)
138  0.00    0.00    -0.00   0.00    0.00    0.00    ).00    0.00    0.00    0.00    0.00    0.00    0.00    {14}:OH_minus#2<->#2+proton(c)
139  Base on reactants/products :
140   gas1        liq1        liq2        liq3
141  1.92e-13    1.92e-13    1.92e-13    1.92e-13    {01}:H20(c)+#1<->OH_minus#1+proton(c)
142  4.32e-01    4.32e-01    4.32e-01    4.32e-01    {02}:OH_minus#1+hole(c)<->OH_rad#1
143  1.35e-01    1.35e-01    1.35e-01    1.35e-01    {03}:OH_rad#1<->0_minus#1+proton(c)
144  1.92e-06    1.92e-06    1.92e-06    1.92e-06    {04}:0_minus#1+0_minus#1<->02_2minus#1+#1
145  2.16e-01    2.16e-01    2.16e-01    2.16e-01    {05}:02_2minus#1+hole(c)<->02_minus#1
146  2.16e-01    2.16e-01    2.16e-01    2.16e-01    {06}:02_minus#1+hole(c)<->02(p)+#1
147  1.50e-19    1.50e-19    1.50e-19    1.50e-19    {07}:#2+hole(c)<->Obr_minus#2
148  7.37e-10    7.37e-10    7.37e-10    7.37e-10    {08}:Obr_minus#2+OH_rad#1<->ObrOH_minus#2+#1
149  1.50e-19    1.50e-19    1.50e-19    1.50e-19    {09}:ObrOH_minus#2+hole(c)<->ObrOH#2
150  6.90e-30    6.90e-30    6.90e-30    6.90e-30    {10}:ObrOH#2<->Obr0_minus#2+proton(c)
151  1.50e-19    1.50e-19    1.50e-19    1.50e-19    {11}:Obr0_minus#2+hole(c)<->02(p)+0vac#2
152  9.44e-34    9.44e-34    9.44e-34    9.44e-34    {12}:H20(c)+0vac#2<->H20#2
153  2.24e-28    2.24e-28    2.24e-28    2.24e-28    {13}:H20#2<->OH_minus#2+proton(c)
154  1.55e-27    1.55e-27    1.55e-27    1.55e-27    {14}:OH_minus#2<->#2+proton(c)
155  Simplification :
156   gas1   liq1   liq2   liq3
157  0.43   0.43   0.43   0.43   {02}:OH_minus#1+hole(c)<->OH_rad#1
158  0.14   0.14   0.14   0.14   {03}:OH_rad#1<->0_minus#1+proton(c)
159  0.22   0.22   0.22   0.22   {05}:02_2minus#1+hole(c)<->02_minus#1
160  0.22   0.22   0.22   0.22   {06}:02_minus#1+hole(c)<->02(p)+#1
161
162  Calculate the degree of rate control of intermediate of species (Q1_02_2minus)
163  Elapsed time: 00:00:00.131. Converged, return with the residue |dy/dt| ~= 10^-1028, |dlog(y)/dt| ~= 10^-1014. Succeed!!
```

关键反应步骤

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输出文件

G:\CATLAB\oxygen evolution reaction\result_WD4\log1_parsum

EDITOR VIEW

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FILE EDIT NAVIGATE BREAKPOINTS

中间体敏感度

```
-0.00  -0.00   0.00   0.00   0.00   0.00  -0.00  -0.00  -0.00  -0.00  -0.00  -0.00  -0.00  -0.00  Q2_ObrO_minus
-0.00  -0.00   0.                                 ).00  -0.00  -0.00  -0.00  -0.00  -0.00  -0.00  Q2_Obr_minus
-0.00  -0.00   0.                                 ).00  -0.00  -0.00  -0.00  -0.00  -0.00  -0.00  Q2_Ovac
-0.00  -0.00   0.00   0.00   0.00   0.00  -1.00  -1.00  -1.00  -1.00  -1.00  -1.00  -1.00  -1.00  Q2_v
Base on reactants/products :
 gas1        liq1        liq2        liq3
-2.16e-01   -2.16e-01   -2.16e-01   -2.16e-01   Q1_O2_2minus
-2.16e-01   -2.16e-01   -2.16e-01   -2.16e-01   Q1_O2_minus
-5.68e-01   -5.68e-01   -5.68e-01   -5.68e-01   Q1_OH_minus
-2.11e-08   -2.11e-08   -2.11e-08   -2.11e-08   Q1_OH_rad
-3.83e-06   -3.83e-06   -3.83e-06   -3.83e-06   Q1_O_minus
-4.00e-06   -4.00e-06   -4.00e-06   -4.00e-06   Q1_v
-2.31e-28   -2.31e-28   -2.31e-28   -2.31e-28   Q2_H2O
-4.65e-21   -4.65e-21   -4.65e-21   -4.65e-21   Q2_OH_minus
-2.11e-29   -2.11e-29   -2.11e-29   -2.11e-29   Q2_ObrOH
-1.50e-19   -1.50e-19   -1.50e-19   -1.50e-19   Q2_ObrOH_minus
-1.50e-19   -1.50e-19   -1.50e-19   -1.50e-19   Q2_ObrO_minus
-1.06e-20   -1.06e-20   -1.06e-20   -1.06e-20   Q2_Obr_minus
-9.44e-34   -9.44e-34   -9.44e-34   -9.44e-34   Q2_Ovac
-7.37e-10   -7.37e-10   -7.37e-10   -7.37e-10   Q2_v
Simplification :
 gas1   liq1   liq2   liq3
-0.22   -0.22   -0.22   -0.22   Q1_O2_2minus
-0.22   -0.22   -0.22   -0.22   Q1_O2_minus
-0.57   -0.57   -0.57   -0.57   Q1_OH_minus

Calculate the degree of rate control of concentration of species (C_H2O)
Elapsed time: 00:00:00.126. Converged, return with the residue |dy/dt| ~= 10^-1028, |dlog(y)/dt| ~= 10^-1018. Succeed!!
Extract individual solutions by numeric::fsolve
0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00   0.00e+00
```

关键中间体

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输出文件

G:\CATLAB\oxygen evolution reaction\result_WD4\log1_parsum

```
Elapsed time: 00:00:00.123. Converged, return with the residue |dy/dt| ~= 10^-1028, |dlog(y)/dt| ~= 10^-1018. Succeed!!
Extract individual solutions by numeric::fsolve
4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22    4.16e-22
Summary :
 R01     R02     R03     R04     R05     R06     R07     R08     R09     R10     R11     R12     R13     R14
 0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00   C_H2O
-1.00   -1.00                                                   -2.00   -2.00   -2.00   -2.00   -2.00   -2.00   C_hole
 0.00    0.00                                                    0.00    0.00    0.00    0.00    0.00    0.00   C_proton
 0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00   P_O2
Base on reactants/products :
 gas1        liq1        liq2        liq3
 0.00e+00    0.00e+00    0.00e+00    0.00e+00    C_H2O
-1.00e+00   -1.00e+00   -1.00e+00   -1.00e+00    C_hole
 0.00e+00    0.00e+00    0.00e+00    0.00e+00    C_proton
 4.16e-22    4.16e-22    4.16e-22    4.16e-22    P_O2
Simplification :
 gas1    liq1    liq2    liq3
-1.00   -1.00   -1.00   -1.00   C_hole

Calculate the degree of rate control of energy descriptor E1
Elapsed time: 00:00:00.127. Converged, return with the residue |dy/dt| ~= 10^-1021, |dlog(y)/dt| ~= 10^-1014. Succeed!!
Extract individual solutions by numeric::fsolve
1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13    1.92e-13
Summary :
 R01     R02     R03     R04     R05     R06     R07     R08     R09     R10     R11     R12     R13     R14
0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    E1
Base on reactants/products :
 gas1        liq1        liq2        liq3
1.92e-13    1.92e-13    1.92e-13    1.92e-13    E1
Simplification :
```

反应物、产物敏感度

关键物种

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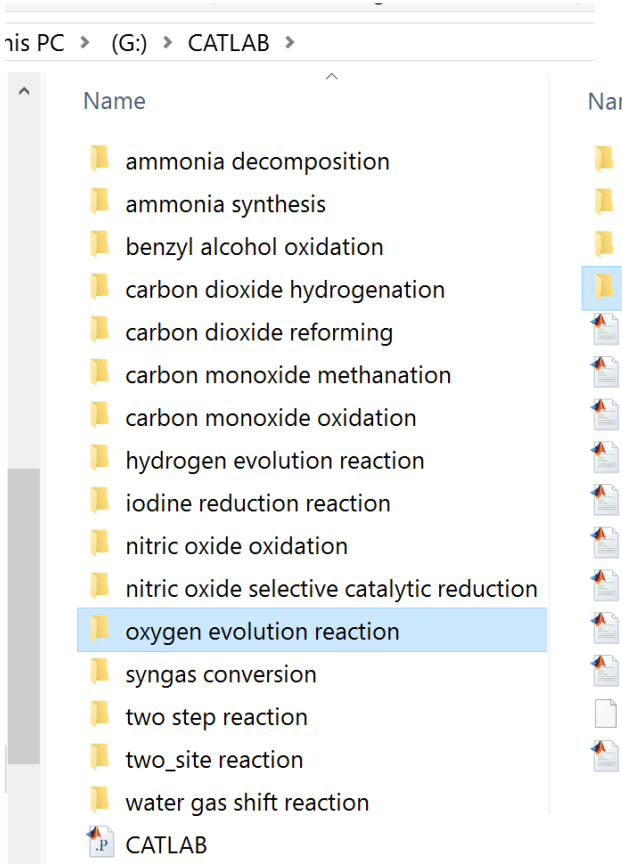
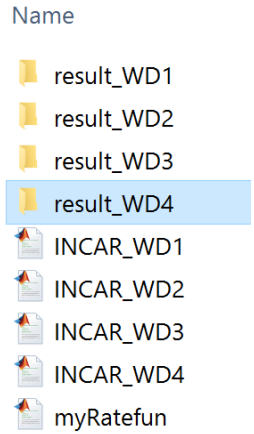
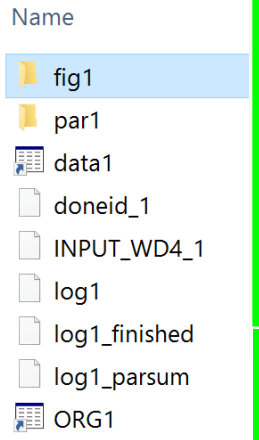
输出文件

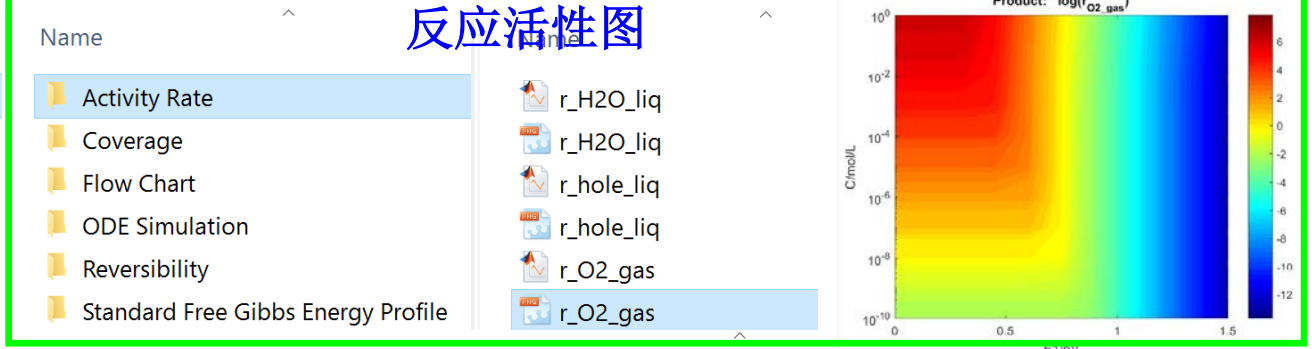




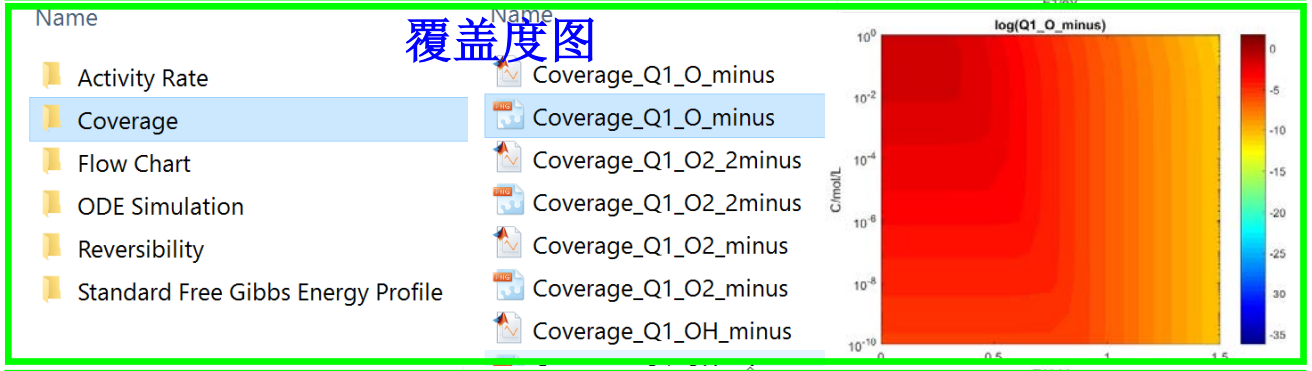


数十个反应类型
数万种模拟条件
数亿次稳态求解

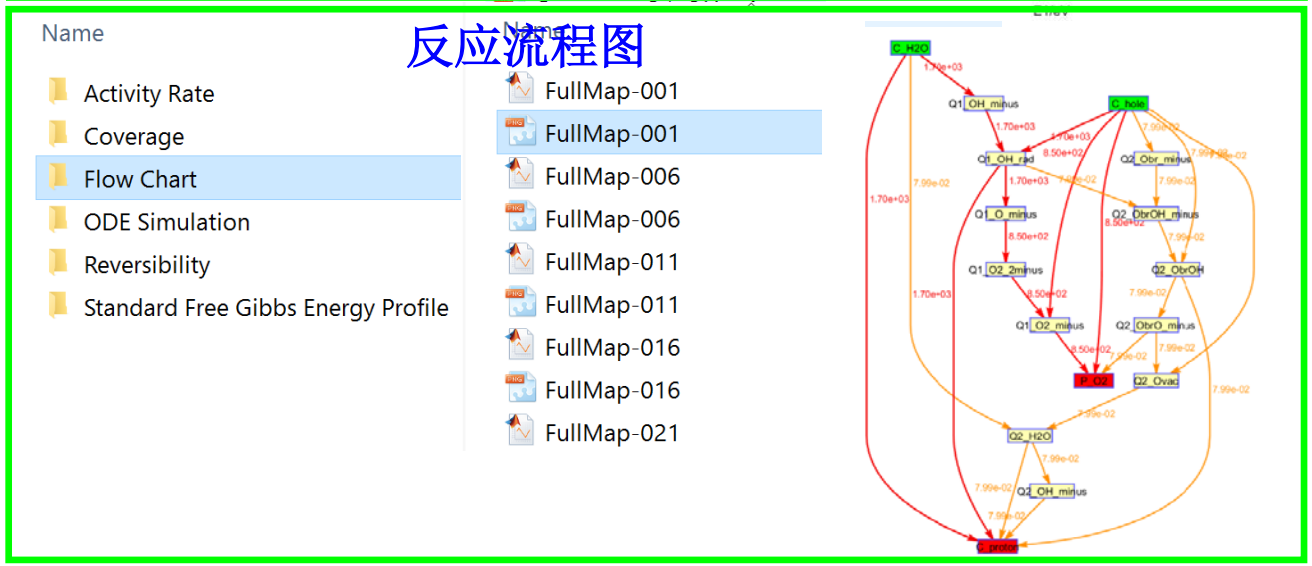
反应活性图



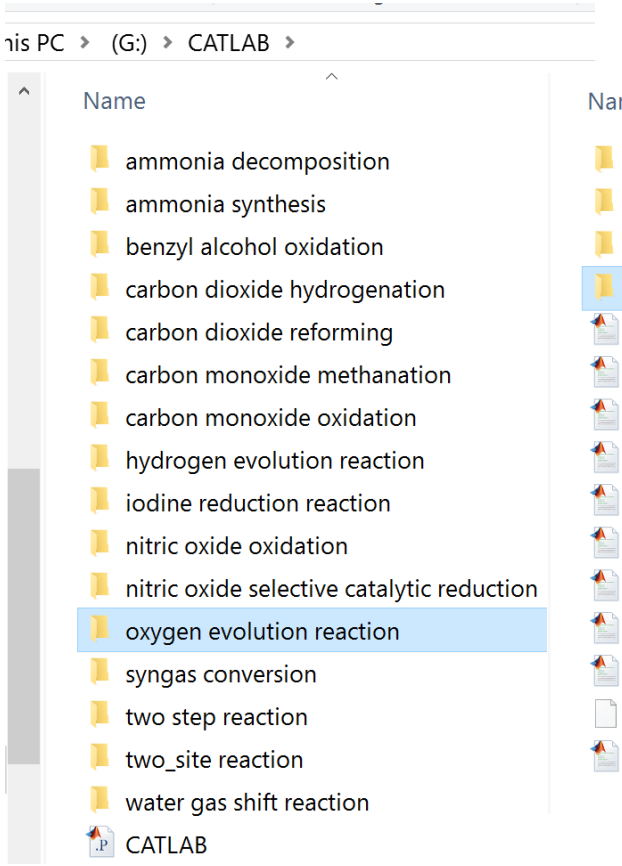
覆盖度图

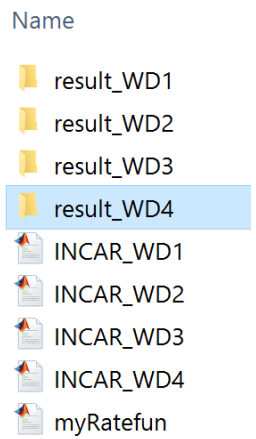


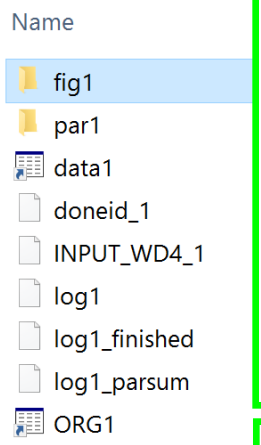
反应流程图



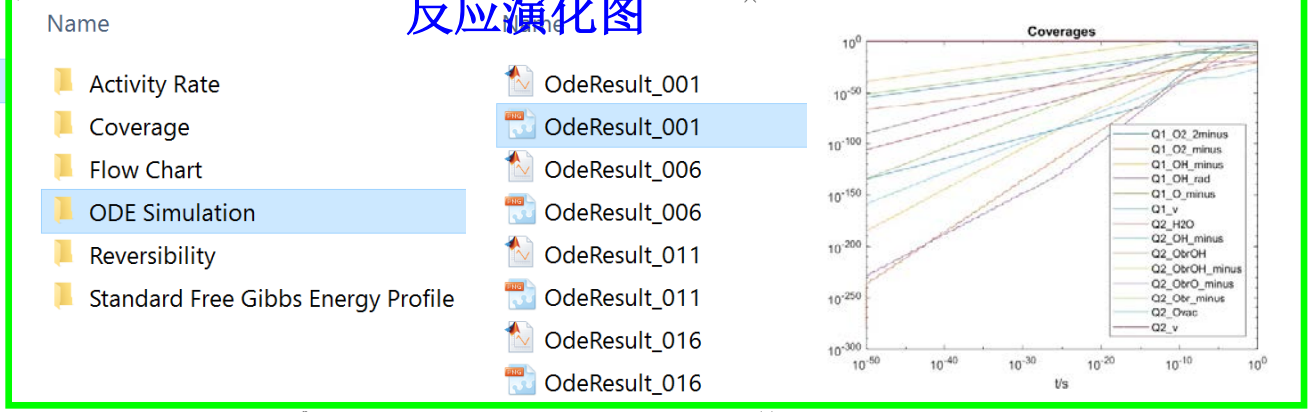
输出文件



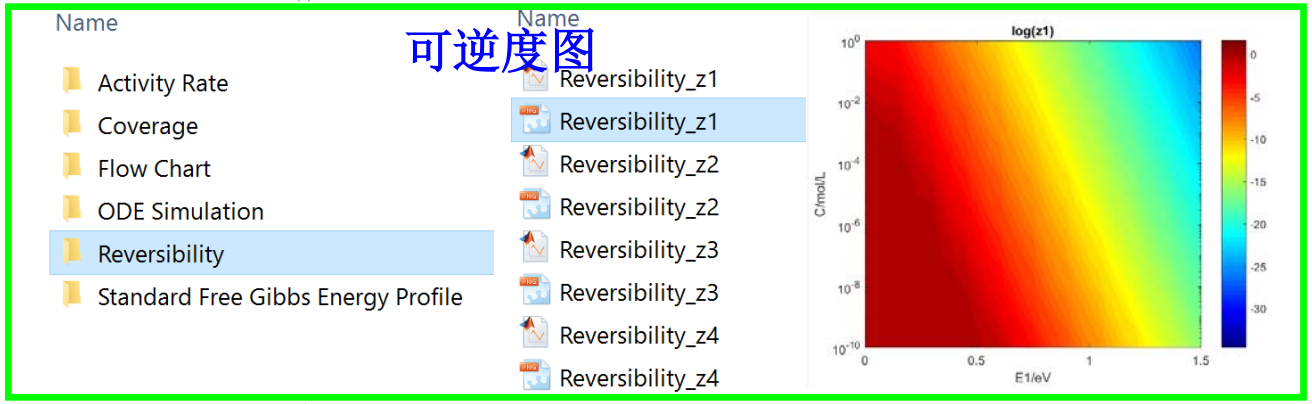




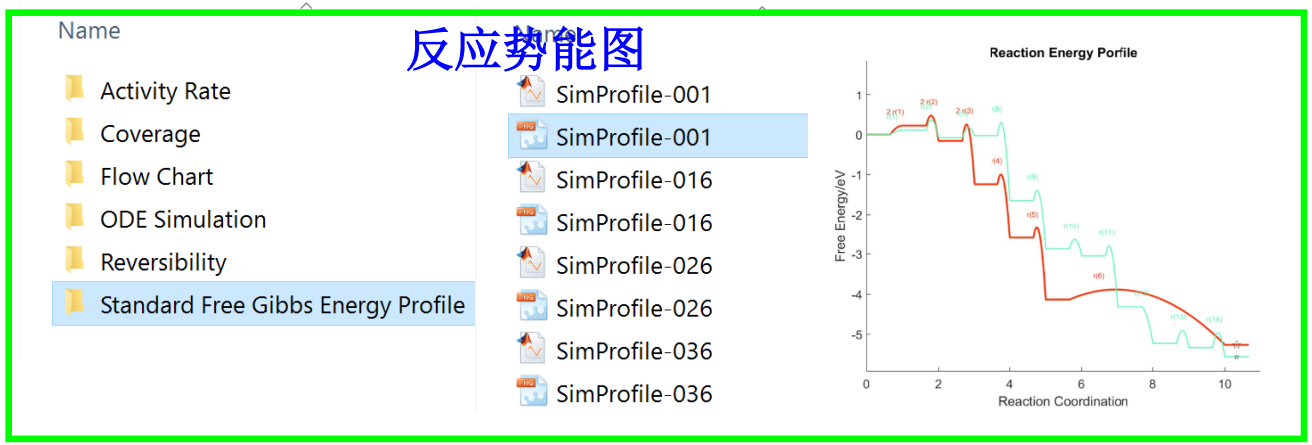
反应演化图



可逆度图



反应势能图



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