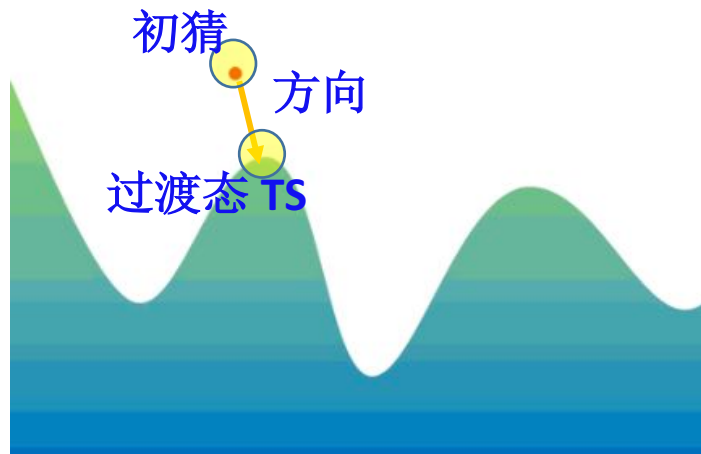


LASP 使用入门4 – 过渡态搜索进阶

猜测过渡态结构和反应方向寻找反应动力学路径

参见 LASP
examples
NN-4

单点行走法
(CBD)



LASP输入文件
lasp.in
input.arc
uncm.arc

lasp.in

关键词

Explore_type **SSW** 选择SSW模块

选择SSW
任务类型

Run_type **1** 晶胞大小固定 适用无周期性分子，团簇
固定晶胞的表面反应

Run_type **11** 晶胞大小可动 适用周期性固体相变（晶体）

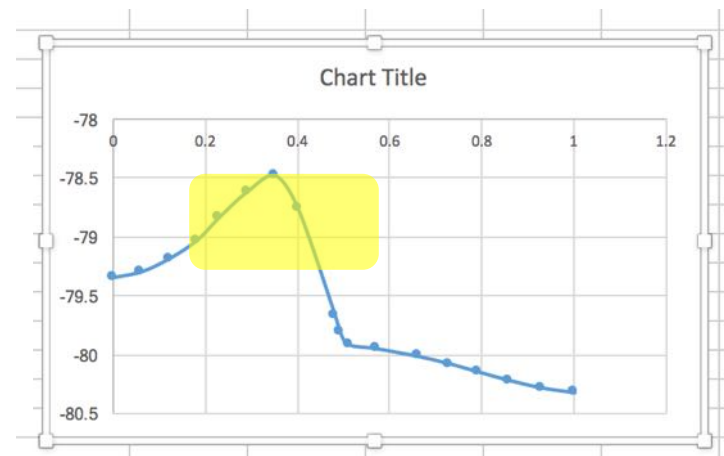
LASP 使用入门4 – 过渡态搜索进阶

构造初始猜测结构三种办法

1. 前期通过两点行走法已经得到了DESW路径，但是没找TS (DESW.task string)，可以利用SSWpath.arc里面的结构。如图，黄色区间对应的结构

2. 知道大概反应机理，通过手动变形初/终态结构

3. 前期搜索过渡态时利用SSW.printevery T
打印了每步的结构，可手动从allstr.arc中间选取类似TS的结构。



一般来说，涉及成断键的过渡态，过渡态键长为成键键长再伸长0.5 Ang左右。比如H₂键长0.7，TS长度一般1.2左右；C-C键长1.4，TS长度经常1.9左右

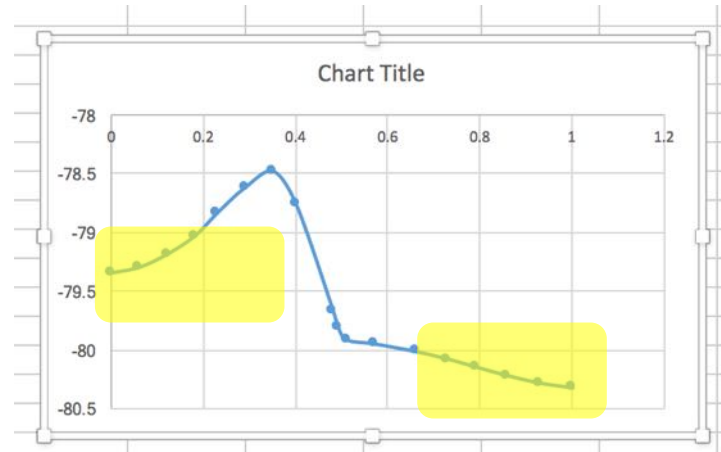
LASP 使用入门4 – 过渡态搜索进阶

构造初始反应方向两种方法

初始反应方向由两个不同结构决定，连续写入`uncm.arc`

1. 前期通过两点行走法已经得到了DESW路径，但是没找TS (DESW.task string)，可以利用SSWpath.arc里面的两边不同结构。如图，两边黄色区对应的结构。

2. 知道大概反应机理，通过手动变形初/终态结构，将变形前和变形后的结构放入



比如，人为拉长C-C键长从1.4到1.8。将前后两帧结构取出

LASP 使用入门4 – 过渡态搜索进阶

总控制关键词

CBD.maxcycle	20	设定优化TS循环数
CBD.maxdist	0.25	设定优化TS单循环中结构最大变化位移 (Ang)
CBD.TSftol	0.1	设定优化TS的收敛精度 (原子最大力 eV/Ang)
CBD.strftol	0.1	设定优化TS的收敛精度 (晶体应力 GPa)
SSW.output	T	设定lasp.out输出的多少
SSW.printevery	T	设定是否输出每一步的结构和力 (对复杂的反应, 建议打开)

LASP 使用入门4 – 过渡态搜索进阶

控制行走方向主要关键词

```
SSW.DimerdR      0.0050
SSW.RotMaxStep_preRot      8
SSW.RotMaxStep      18
SSW.Rotftol_preRot      1.0000
SSW.Rotftol      0.1000
```

控制双子优化mode精度

- 利用约束旋转双子法（**CBD**）优化行走方向

SSW.Rotftol **0.01 ~ 0.1**

SSW.Rotftol_preRot **0.5~1.0**

对于虚频接近0的TS（soft TS），
可以尝试改小SSW.Rotftol

LASP 使用入门4 – 过渡态搜索进阶

准备输入结构文件 uncm.arc; input.arc; lasp.in (其他为和PES相关文件)

```

7:47:24:[zpliu@console NN-4]$ ll
total 52K
-rwxrwxrwx 1 zpliu zpliu 18 Jun 4 17:39 uncm.arc -> sourcedir/uncm.arc
-rwxrwxrwx 1 zpliu zpliu 17 Jun 4 17:39 lasp.in -> sourcedir/lasp.in
-rwxrwxrwx 1 zpliu zpliu 19 Jun 4 17:39 input.arc -> sourcedir/input.arc
-rw-r--r-- 1 zpliu zpliu 938 Jun 4 17:39 sge.script
-rw-rw-r-- 1 zpliu zpliu 0 Jun 4 17:39 output
-rwxrwxrwx 1 zpliu zpliu 18 Jun 4 17:41 CHON.pot -> sourcedir/CHON.pot
-rwxr-xr-x 2 zpliu zpliu 4.0K Jun 4 17:42 sourcedir/
-rw----- 1 zpliu zpliu 0 Jun 4 21:33 nohup.out
-rw-r--r-- 1 zpliu zpliu 3.1K Jun 4 21:33 allkeys.log
-rw-r--r-- 1 zpliu zpliu 1.4K Jun 4 21:33 TSstr.arc
-rw-r--r-- 1 zpliu zpliu 22K Jun 4 21:33 TSmode.arc
-rw-r--r-- 1 zpliu zpliu 12K Jun 4 21:33 lasp.out
    
```

input.arc 文件里面有一个结构，是猜测的过渡态

uncm.arc

文件里面有两个结构（不一定是优化过的），结构的变化指明反应的方向（注意：原子需要一一对应

用户自己做uncm.arc: 可以利用MS画结构，并存为car文件格式，贴到uncm.arc

```

17:48:23:[zpliu@console NN-4]$ cat uncm.arc
BIOSYM archive 2
PBC=ON
  React 1 1 -1335.4875956 -1335.4875956
IDATE
PBC 15.0000 15.0000 15.0000 90.0000 90.0000 90.0000
H 3.144160760 4.517488769 6.756447451 CORE 1 H H 0.0000 1
H 3.283939812 2.651288474 6.678731676 CORE 2 H H 0.0000 2
H 5.596489157 2.869418544 5.804940015 CORE 3 H H 0.0000 3
H 6.663678005 5.186591815 5.762493313 CORE 4 H H 0.0000 4
H 5.125262368 5.906143482 6.339914284 CORE 5 H H 0.0000 5
H 2.125315930 4.905870300 3.098265313 CORE 6 H H 0.0000 6
H 3.575335246 3.710735357 3.102529396 CORE 7 H H 0.0000 7
H 3.523704793 6.570586555 4.359380806 CORE 8 H H 0.0000 8
C 5.018270423 3.760641652 6.078727728 CORE 9 C C 0.0000 9
C 3.915436135 5.595886110 4.027892549 CORE 10 C C 0.0000 10
C 3.157740732 4.682453702 3.375488562 CORE 11 C C 0.0000 11
C 3.750282281 3.630455282 6.543086063 CORE 12 C C 0.0000 12
C 5.566495745 5.117793255 5.703135701 CORE 13 C C 0.0000 13
O 5.266654611 5.386893703 4.285289141 CORE 14 O 0 0.0000 14
end
  React 1 2 -1335.4875956 -1336.5710057
IDATE
PBC 15.0000 15.0000 15.0000 90.0000 90.0000 90.0000
H 3.144160760 4.517488769 6.756447451 CORE 1 H H 0.0000 1
H 3.010391122 3.101706762 5.934107924 CORE 2 H H 0.0000 2
H 5.463107657 2.875164776 5.735325439 CORE 3 H H 0.0000 3
H 6.873034983 4.546433673 6.800129624 CORE 4 H H 0.0000 4
H 5.451696901 5.762263561 6.872310103 CORE 5 H H 0.0000 5
H 2.234067776 4.235094530 3.947014943 CORE 6 H H 0.0000 6
H 3.860660375 3.615131427 3.505464637 CORE 7 H H 0.0000 7
H 3.216976521 6.522536252 4.451976265 CORE 8 H H 0.0000 8
C 5.023626124 3.841727937 6.014177473 CORE 9 C C 0.0000 9
C 3.759024520 5.740272560 3.850574344 CORE 10 C C 0.0000 10
C 3.318979905 4.317934153 4.156960399 CORE 11 C C 0.0000 11
C 3.556447807 4.024611797 5.673831366 CORE 12 C C 0.0000 12
C 5.820569016 4.768449809 6.599616539 CORE 13 C C 0.0000 13
O 4.651214584 6.062278980 3.059462504 CORE 14 O 0 0.0000 14
end
end
    
```


LASP 使用入门4 – 过渡态搜索进阶

查看结果 [lasp.out](#) 检索TS得到CBD 寻找TS轨迹

```

17:49:54:[zpliu@console NN-4]$ grep TS lasp.out
Start to Construct TS class
TS-seach-Energy, force      -78.561114834      0.65
TS-seach-Energy, force      -78.557231575      0.64
TS-seach-Energy, force      -78.556735604      0.64
TS-seach-Energy, force      -78.556562902      0.64
TS-seach-Energy, force      -78.555932690      0.63
TS-seach-Energy, force      -78.555692989      0.63
TS-seach-Energy, force      -78.555700400      0.63
TS-seach-Energy, force      -78.555648234      0.63
TS-seach-Energy, force      -78.561114834      0.65
TS-seach-Energy, force      -78.533794316      0.58
TS-seach-Energy, force      -78.538238739      0.64
TS-seach-Energy, force      -78.537249844      0.39
TS-seach-Energy, force      -78.543642307      0.30
TS-seach-Energy, force      -78.545546588      0.32
TS-seach-Energy, force      -78.550009946      0.36
TS-seach-Energy, force      -78.552632231      0.20
TS-seach-Energy, force      -78.544829073      0.69
TS-seach-Energy, force      -78.555627652      0.41
TS-seach-Energy, force      -78.505154513      2.10
TS-seach-Energy, force      -78.555627652      0.41
TS-seach-Energy, force      -78.555106322      0.41
TS-seach-Energy, force      -78.554953797      0.43
TS-seach-Energy, force      -78.555167519      0.40
TS-seach-Energy, force      -78.555083154      0.41
TS-seach-Energy, force      -78.555165805      0.41
TS-seach-Energy, force      -78.555111273      0.41
TS-seach-Energy, force      -78.555627652      0.41
TS-seach-Energy, force      -78.512667109      1.94
TS-seach-Energy, force      -78.561478983      0.26
TS-seach-Energy, force      -78.548745624      1.10
TS-seach-Energy, force      -78.565725609      0.12
TS-seach-Energy, force      -78.563899768      0.48
TS-seach-Energy, force      -78.568792026      0.24
TS-seach-Energy, force      -78.566601251      0.65
TS information      -78.571856 -5.789581 0.095476 0.000000 0.000000
TS-seach-Energy, force      -78.571856080      0.10

```

找准反应mode

(energy/force 基本不变)

朝TS优化结构

(energy 趋势性变低, force 趋势性变小)

TS原子最大力

TS虚频率值

TS能量

LASP 使用入门4 – 过渡态搜索进阶

查看结果 [lasp.out](#) 检索Curv得到CBD 寻找TS轨迹中
关于频率的信息

```

17:51:33:[zpliu@console NN-4]$ grep Curv lasp.out
Curv real -4.50485356102658
CBD_Rotate: Fv,ftol,Curv 1 0.537169 1.000000 -4.504854 -4.504854
Curv real -7.31724313999570
CBD_Rotate: Fv,ftol,Curv 2 0.449970 0.100000 -7.317243 -7.317243
Curv real -8.47138507457987
CBD_Rotate: Fv,ftol,Curv 3 0.385950 0.100000 -8.471385 -8.471385
Curv real -11.8552455379357
CBD_Rotate: Fv,ftol,Curv 4 0.241695 0.100000 -11.855246 -11.855246
Curv real -13.1117479994517
CBD_Rotate: Fv,ftol,Curv 5 0.109170 0.100000 -13.111748 -13.111748
Curv real -13.0737426975446
CBD_Rotate: Fv,ftol,Curv 6 0.115464 0.100000 -13.073743 -13.073743
Curv real -13.3672977991485
CBD_Rotate: Fv,ftol,Curv 7 0.030203 0.100000 -13.367298 -13.367298
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 1.1268 0.8618
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 0.5539 1.3398
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 0.5224 1.0654
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 0.3873 1.0405
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 0.2929 0.6668
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 0.2131 0.8398
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 0.1755 0.7000
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 0.1686 0.4456
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 0.1353 1.6320
Translation at Curv < 0 -13.36730, F=Fv-Lamda*FN, FN 1.0000 0.1142 0.8051
Curv real -3.94441884178487
CBD_Rotate: Fv,ftol,Curv 1 0.269116 1.000000 -3.944419 -3.944419
Curv real -4.47941619032063
CBD_Rotate: Fv,ftol,Curv 2 0.383028 0.100000 -4.479416 -4.479416
Curv real -5.07743541571001
CBD_Rotate: Fv,ftol,Curv 3 0.212366 0.100000 -5.077435 -5.077435
Curv real -5.42239192974899
CBD_Rotate: Fv,ftol,Curv 4 0.141156 0.100000 -5.422392 -5.422392
Curv real -5.69947324410195
CBD_Rotate: Fv,ftol,Curv 5 0.138501 0.100000 -5.699473 -5.699473
Curv real -5.78958057278538
CBD_Rotate: Fv,ftol,Curv 6 0.067984 0.100000 -5.789581 -5.789581
Translation at Curv < 0 -5.78958, F=Fv-Lamda*FN, FN 1.0000 0.1178 0.8046
Translation at Curv < 0 -5.78958, F=Fv-Lamda*FN, FN 1.0000 0.0802 3.2411
Translation at Curv < 0 -5.78958, F=Fv-Lamda*FN, FN 1.0000 0.0855 0.5050
Translation at Curv < 0 -5.78958, F=Fv-Lamda*FN, FN 1.0000 0.0687 1.8627
Translation at Curv < 0 -5.78958, F=Fv-Lamda*FN, FN 1.0000 0.0593 0.3710
Translation at Curv < 0 -5.78958, F=Fv-Lamda*FN, FN 1.0000 0.0404 1.0046
Translation at Curv < 0 -5.78958, F=Fv-Lamda*FN, FN 1.0000 0.0418 0.4582
Translation at Curv < 0 -5.78958, F=Fv-Lamda*FN, FN 1.0000 0.0294 1.0531

```

找准反应mode

Cycle-1

朝TS优化结构

找准反应mode

Cycle-2

朝TS优化结构

LASP 使用入门4 – 过渡态搜索进阶

查看结果

查看结构

TSstr.arc

TS结构

TSmode.arc

TS 对应反应虚频的结构动画

利用Material Studio 查看arc文件，可动画放映！

