

## ReaxFF MD 局部区域反应追踪与物理性质可视化分析

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## Visualized Reaction Tracking and Physical Property Analysis for a Picked 3D Area in a Reactive Molecular Dynamics Simulation System

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煤颗粒体系特征反应列表与其 2D 结构

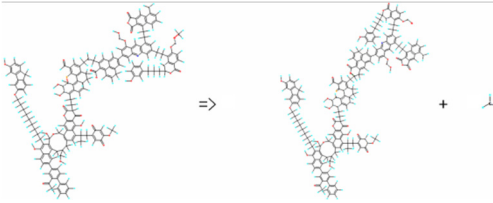
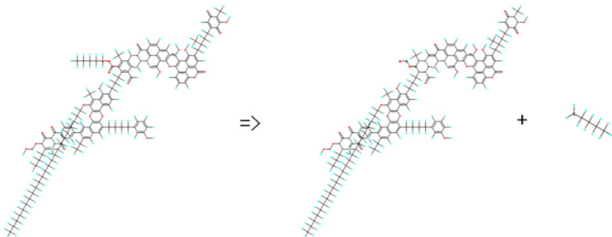
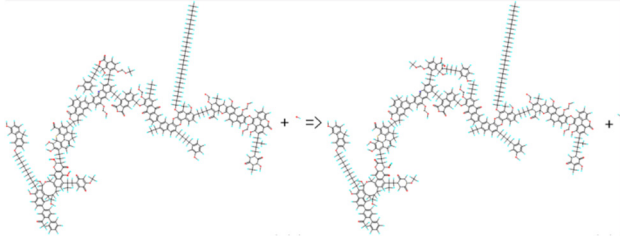
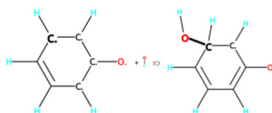
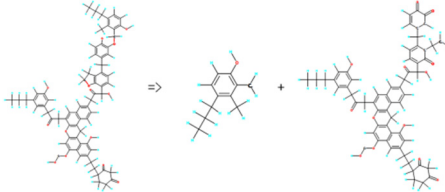
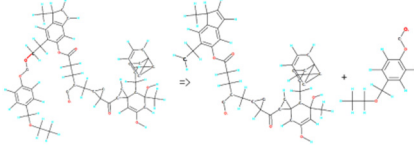
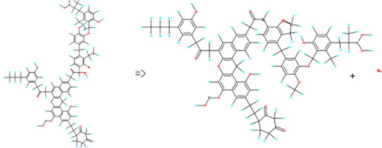
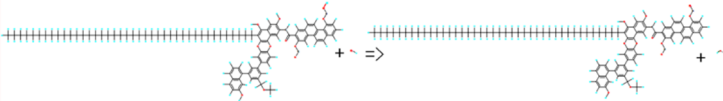
表 S1 5–205 ps 模拟时间内煤颗粒体系特征化学反应列表及其 2D 结构

Table S1 Examples of characteristic reaction of coal particle system and its 2D structure during 5–205 ps.

No.	Time (ps)	Reaction list and structure view in 2D
1	5–15	$\text{H} + \text{C}_7\text{H}_6 \rightarrow \text{C}_7\text{H}_5 + \text{H}_2$
2	15–25	$\text{C}_{73}\text{H}_{70}\text{O}_{16} \rightarrow \text{C}_{12}\text{H}_{15}\text{O}_3 + \text{C}_{61}\text{H}_{55}\text{O}_{13}$
3	15–25	$\text{C}_{105}\text{H}_{96}\text{O}_{20}\text{S} \rightleftharpoons \text{C}_{99}\text{H}_{91}\text{O}_{19}\text{S} + \text{C}_6\text{H}_5\text{O} \text{ (reversible)}$
4	25–35	$\text{C}_{65}\text{H}_{55}\text{O}_{13} \rightarrow \text{C}_{65}\text{H}_{55}\text{O}_{13} \text{ (structure transformation)}$
5	25–35	$\text{C}_{164}\text{H}_{152}\text{O}_{33} \rightarrow \text{C}_{73}\text{H}_{71}\text{O}_{14} + \text{C}_{91}\text{H}_{81}\text{O}_{19}$
6	35–45	$\text{C}_{73}\text{H}_{70}\text{O}_{16} \rightarrow \text{C}_{61}\text{H}_{55}\text{O}_{13} + \text{C}_{12}\text{H}_{14}\text{O}_2 + \text{HO}$
7	35–45	$\text{C}_{20}\text{H}_{24}\text{O}_2 \rightarrow \text{C}_{13}\text{H}_{10}\text{O}_2 + \text{C}_7\text{H}_{14}$

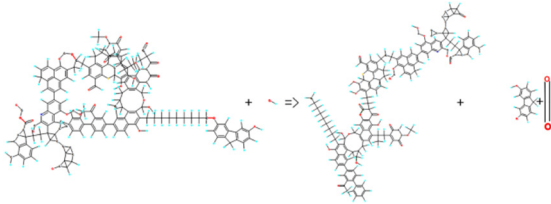
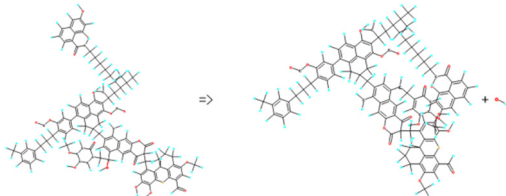
to be continued

continued Table S1

No.	Time (ps)	Reaction list ad & structure view in 2D
8	45–55	$\text{C}_{164}\text{H}_{133}\text{O}_{29}\text{NS} \rightarrow \text{C}_{163}\text{H}_{130}\text{O}_{29}\text{NS} + \text{CH}_3$ 
9	45–55	$\text{C}_{135}\text{H}_{137}\text{O}_{26} \rightarrow \text{C}_{130}\text{H}_{126}\text{O}_{26} + \text{C}_5\text{H}_{11}$ 
10	65–75	$\text{C}_{294}\text{H}_{261}\text{O}_{56}\text{NS} + \text{HO} \rightarrow \text{C}_{294}\text{H}_{260}\text{O}_{56}\text{NS} + \text{H}_2\text{O}$ 
11	75–80	$\text{C}_6\text{H}_5\text{O} + \text{HO} \rightarrow \text{C}_6\text{H}_6\text{O}_2$ 
12	75–85	$\text{C}_{71}\text{H}_{67}\text{O}_{14} \rightarrow \text{C}_{60}\text{H}_{52}\text{O}_{13} + \text{C}_{11}\text{H}_{15}\text{O}$ 
13	75–85	$\text{C}_{53}\text{H}_{44}\text{O}_9 \rightarrow \text{C}_{43}\text{H}_{33}\text{O}_6 + \text{C}_{10}\text{H}_{11}\text{O}_3$ 
14	115–125	$\text{C}_{73}\text{H}_{71}\text{O}_{16} \rightarrow \text{C}_{73}\text{H}_{70}\text{O}_{15} + \text{HO}$ 
15	115–125	$\text{C}_{96}\text{H}_{114}\text{O}_{11} + \text{HO} \rightarrow \text{H}_2\text{O} + \text{C}_{96}\text{H}_{113}\text{O}_{11}$ 

to be continued

continued Table S1

No.	Time (ps)	Reaction list ad & structure view in 2D
16	155–165	$\text{C}_{154}\text{H}_{111}\text{O}_{25}\text{NS} + \text{HO} \rightarrow \text{CO}_2 + \text{C}_{140}\text{H}_{103}\text{O}_{22}\text{NS} + \text{C}_{13}\text{H}_9\text{O}_2$ 
17	165–175	$\text{C}_{105}\text{H}_{95}\text{O}_{20}\text{S} \rightarrow \text{CO}_2 + \text{C}_6\text{H}_5\text{O} + \text{C}_{98}\text{H}_{90}\text{O}_{17}\text{S}$ 

### VARxMD 扩展的区域原子 MSD 算法

目前 VARxMD 的全局 MSD 分析功能算法的输入条件有三个：起始时间  $t_s$ ，终止时间  $t_e$ ，粒子集合  $A_s$ 。其中全局的 MSD 功能的分析粒子集合对象主要为三种：在  $t_s-t_e$  之间不发生反应的物种、所有原子、选择元素类型的原子。同理，区域的 MSD 分析功能也是可以计算区域中选择粒子在生命周期内从起始时间  $t_s$  到终止时间  $t_e$  的位移偏差的平均，从而定性判断局部区域粒子的扩散现象。但是由于区域中所选择分子的寿命在  $t_s-t_e$  时间段下的不相同，并不可简单获得；若要获取区域分子的 MSD 性质，必须首先要统计每个不同区域分子的时间寿命，再在分子时间寿命内分析区域分子的 MSD。因此，目前区域的 MSD 只可针对所有原子、选择元素类型的原子做计算。

关于 MSD 的程序实现与 RDF 大致相同，主要分为两部分：MSD 的数据结构部分和计算函数部分。其中 MSD 数据结构主要由时间  $t$  动态数组和结果  $msd$  动态数组组成，即如图 S1a 所示；计算函数功能需要已知起始时间和终止时间下的所选择原子的坐标位置，输出为 MSD 结果数据，具体算法伪代码实现如下图 S1b 所示。

```

Struct MSD{           (a)
std::vector<double> t;
std::vector<double> msd;
};

Algorithm: MSD of picked atoms  $A_s$  during start time  $t_s$  and end time  $t_e$ . (b)
Input: start time  $t_s$  and end time  $t_e$ .
Output: MSD vector.
Steps:
1) Initialize time  $t$  vector and  $msd$  vector of MSD,  $n_A$  is number of  $A_s$ .
2) Define count vector  $cnt$  and vector of x, y, z direction distance  $sdx, sdy, sdz$ .
3) For  $t_1$  in  $[t_s, t_e]$ :
For  $dt$  in  $[0, t_e - t_s]$ :
 $cnt[dt]++$ ,  $t_2 = t_1 + dt$ .
For  $A$  in  $A_s$ :
 $dx = X_{At2} - X_{At1}, dy = Y_{At2} - Y_{At1}, dz = Z_{At2} - Z_{At1}$ 
 $sdx[dt] += dx^2, sdy[dt] += dy^2, sdz[dt] += dz^2$ 
4) For  $dt$  in  $[0, t_e - t_s]$ :
 $sdx[dt] = \frac{sdx[dt]}{n_A cnt[dt]}, sdy[dt] = \frac{sdy[dt]}{n_A cnt[dt]}, sdz[dt] = \frac{sdz[dt]}{n_A cnt[dt]}$ 
Add  $dt$  to  $t$  vector of MSD.
Add  $sdx + sdy + sdz$  to  $msd$  vector of MSD.
Return MSD.

```

图 S1 VARxMD 扩展的局部区域原子的 MSD 算法伪代码：(a)数据结构(b)计算部分

Fig. S1 Atom MSD algorithm pseudo code for a picked area in VARxMD extension (a) data structure (b) calculation part.