“Following the experimental immersion operation, MIL-101(Cr) was immersed in aqueous solutions containing different amounts of LiCl (i.e., 0.91 wt%, 1.80 wt%, 4.37 wt%, and 8.38 wt %), and then water molecules were gradually evaporated from the solution. Such a process was simulated by molecular dynamics (MD) simulation using the GROMACS package [27]. After immersing MIL-101(Cr) in a box of LiCl solutions containing 10, 20, 50 and 100 ion pairs, respectively….”

Ref:

*International journal of hydrogen energy* ,2023,48,18366e18374

本次计算以0.91Wt%为例展开计算



将*m*(LiCl)视为*m*1，*m*(MOF)视为*m*2，对式1.1进行展开如式1.2所示：





*m*2的质量为MOF的质量，此时的体积的应该是盒子的体积175465立方埃，该数据源于MS自动计算。





上式的A为Å，且1 cm3= 1024 Å3 ，



则：



又因为：



*N*A=6.023×1023 ，*M*1为LiCl的相对原子质量取42.39，则*N*1为：



Table 1 LiCl离子数

|  |  |  |  |
| --- | --- | --- | --- |
| 0.91wt% | 1.80wt% | 4.37wt% | 8.38wt% |
| 10.068 | 20.095 | 50.098 | 100.275 |

所以综上所述，所得公式如下：

X为质量分数，M为溶质分子的相对原子质量，g/mol；m为MOF的质量，g。

