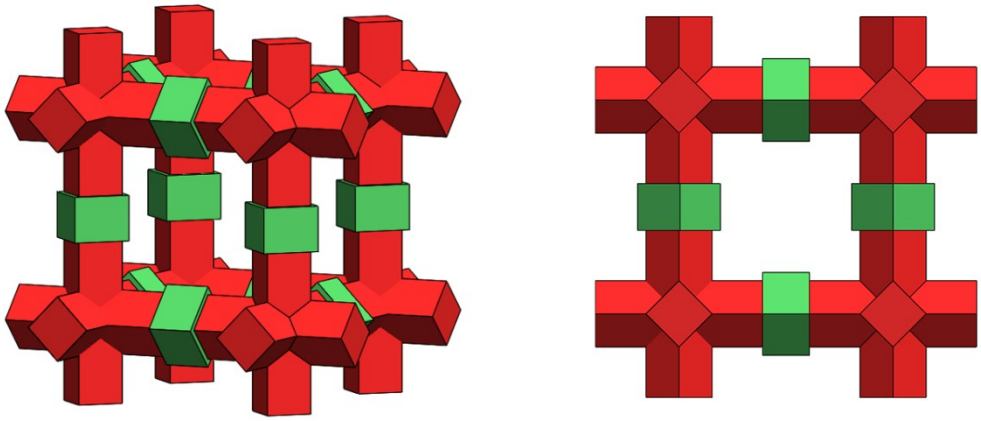
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The simplified structure and the distribution of attractive regions

In this material, we use IRMOF-1 as an example to explain the distribution of the attractive regions. For other materials discussed in our paper, the structures and the distributions of attractive regions are similar.

1. The simplified structure of IRMOF-1.



(a) The overall simplified structure (b) The front view of the simplified structure

Fig. 1 The simplified structure of IRMOF-1

In Fig. 1, the red parts represent the corners, the green parts represent the linkers.

2. The distribution of the attractive regions.

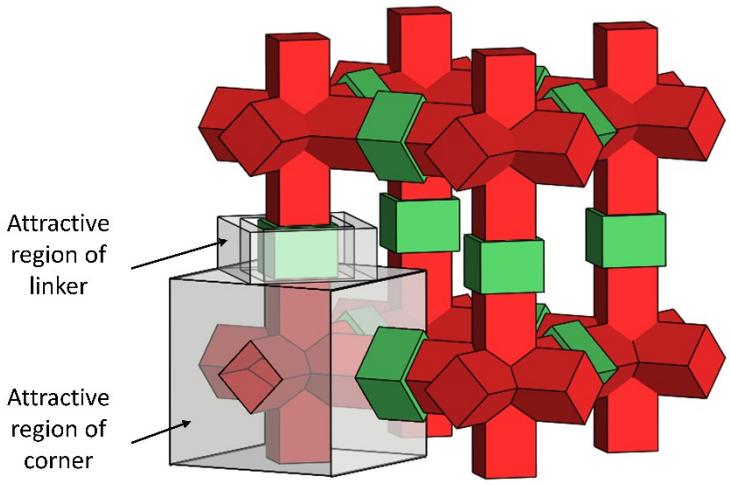


Fig. 2 The locations of the attractive regions

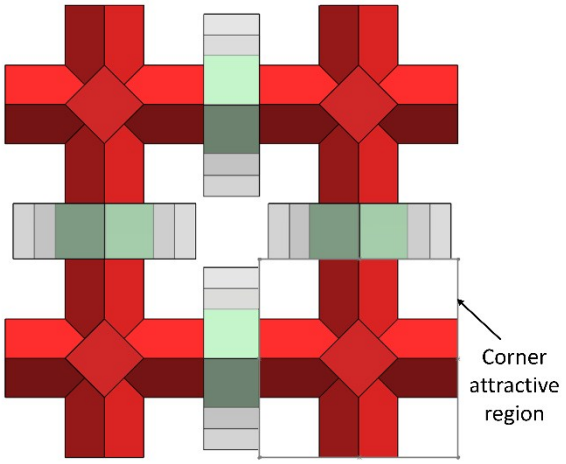
Fig. 2 shows the location of the attractive regions for one corner and one linker. For the other corners and linkers, their attractive regions are exactly the same in shapes and sizes as these two. Since the

attractive region of the corner is cubic in shape and the size is fixed, it is not possible that the attractive regions of different corners overlap. Fig. 2 also shows that it is impossible for the attractive region of linkers to overlap with that of corners.

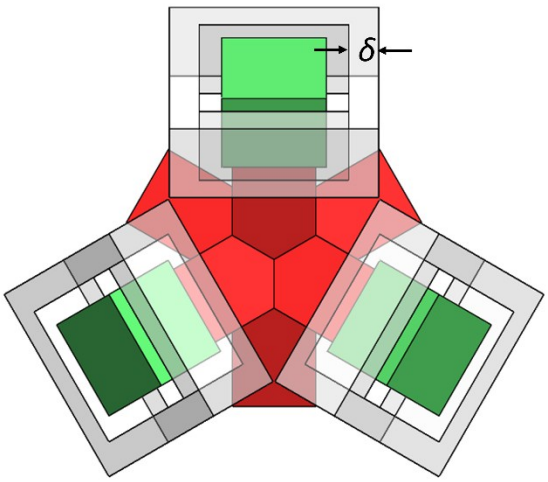
3. The cases when attractive regions overlap

Fig. 3 to 5, further prove that the attractive region at the corner will not overlap with any other regions. For the attractive regions of the linkers, as the width of the attractive region (δ) increases, the overlaps will become more and more complicated in shapes. The three cases shown below depict the change in the overlapping condition of the attractive regions of linkers as δ increases.

Case 1: No overlap



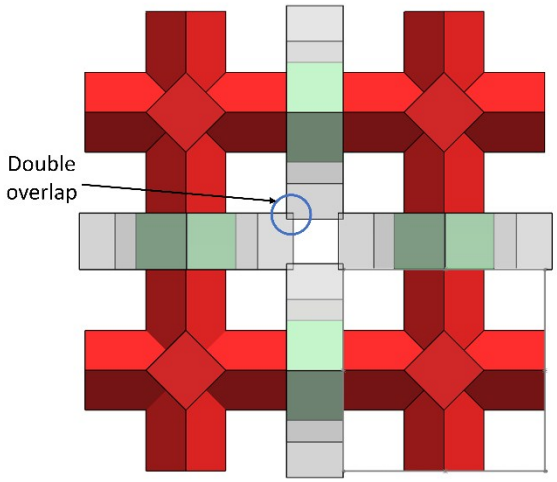
(a) Front view of attractive regions



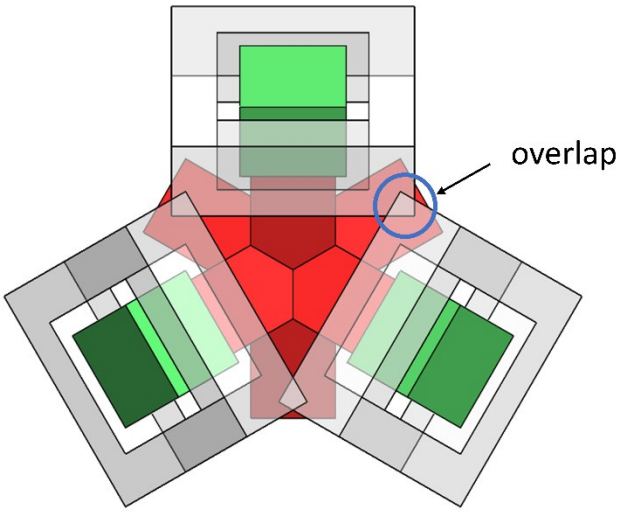
(b) Linkers' attractive regions (view from a vertex)

Fig. 3 Distribution of attractive regions when there is no overlap

Case 2: Double overlap



(a) Front view of the attractive regions

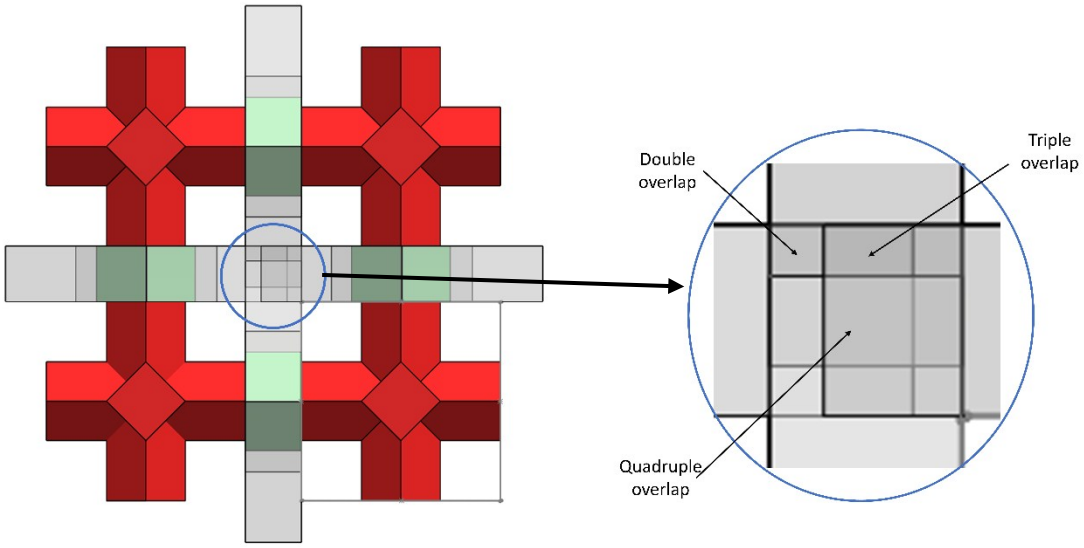


(b) Linkers' attractive regions (view from a vertex)

Fig. 4 Distribution of the attractive regions when double overlaps happen.

Fig. 4 describe the case when double overlap happens. As shown in Fig. 4 (b), double overlaps only happen at the corner of the linkers' attractive regions. The rest of the linkers' attractive regions are non-overlapping regions.

Case 3: Triple and quadruple overlaps.



(a) (b)

Fig. 5 Distribution of the attractive regions when triple and quadruple overlaps happen.

There are two places where triple overlaps can happen. It is possible that when the value of δ is large, the three attractive regions of the linkers in Fig. 4 (b) overlap and form triple overlap. Fig. 5 shows another place where triple overlap happens. At the same time, quadruple overlap will also happen when the triple overlap in Fig.5 happens.

The three cases listed above are just simple examples. If the value of δ keep increasing, more complicated overlapped regions will appear. Therefore, we control the range of δ to avoid these cases. In this work, we control the value of δ, such that only case 1 or case 2 happens.