Accommodation of a dimer in an Ar-like lattice: exploring the generic structural motifs

Georgiy K. Ozerov, Dmitry S. Bezrukov, and Alexei A. Buchachenko

Supplementary Information

Typical Structures of Stable Atomic Trapping Sites

Typical structures are presented in order of increasing \( N_0 \), the number of host atoms removed from the crystal. For each \( N_0 \), the representative site structures are shown with the reference to clustering map discussed in the main text. The area populated by the structures of certain type is given as the percentage of the whole map area. Dominant symmetry of host environment with respect to atom and dimer center (T, O, C for tetrahedral, octahedral, and cuboctahedral, respectively) is provided as established by the radial distribution function analysis (see main text). The ranges of the minimum distances between guest and host atoms \( r_{GH} \) are also shown in units of lattice parameter.

In the structure plots, guest atoms are shown in red together with the first coordination polyhedron. Host atoms composing the first coordination polyhedron are shown in blue, the rest — in gray. Arrows at the bottom-left indicate \( x, y, z \) ideal lattice vectors of the length \( a/2 \).

<table>
<thead>
<tr>
<th>map/region representative structures</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_0 = 0 )</td>
</tr>
<tr>
<td>6%, atom symmetry:Td,100%T, ( r_{GH} \in [0.41, 0.45] )</td>
</tr>
</tbody>
</table>

\[
\begin{array}{cc}
\rho (\text{Å}) & \epsilon (\text{cm}^{-1}) \\
\hline
1 & 10^4 \\
2 & 10^3 \\
3 & 10^2 \\
4 & 10 \\
5 & 10 \\
6 & 10 \\
7 & 10 \\
\end{array}
\]

\[
\begin{array}{cc}
\rho (\text{Å}) & \epsilon (\text{cm}^{-1}) \\
\hline
1 & 10^4 \\
2 & 10^3 \\
3 & 10^2 \\
4 & 10 \\
5 & 10 \\
6 & 10 \\
7 & 10 \\
\end{array}
\]

27\%, atom symmetry:Oh,100%O, \( r_{GH} \in [0.45, 0.57] \)

<table>
<thead>
<tr>
<th>( N_0 = 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_0 = 1 )</td>
</tr>
</tbody>
</table>

1
41%.  atom symmetry: $O_h$, $96\%$ C, $r_{GH} \in [0.63, 0.82]$  

$N_0 = 4$  
16%.  atom symmetry: $T_d$, $99\%$ T, $r_{GH} \in [0.83, 0.92]$  

$N_0 = 6$  
10%.  atom symmetry: $O_h$, $96\%$ O, $r_{GH} \in [0.91, 1.06]$
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Supplementary Information

Typical Structures of Stable Dimer Trapping Sites: Model I

Typical structures are presented in order of increasing \( N_0 \), the number of host atoms removed from the crystal. For each \( N_0 \), the representative site structures are shown with the reference to clustering map discussed in the main text. The area populated by the structures of certain type is given as the percentage of the whole map area. Dominant symmetry of host environment with respect to atom and dimer center (T, O, C for tetrahedral, octahedral, and cuboctahedral, respectively) is provided as established by the radial distribution function analysis (see main text). The ranges of the minimum distances between guest and host atoms \( r_{GH} \) and distances between guest atoms \( r_{GG} \) are also shown in units of lattice parameter.

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<th>representative structures</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_0 = 1 )</td>
<td>9%; atom symmetry: ( O_h ), 97%; center symmetry: ( O_h ), 100%; ( r_{GH} \in [0.61, 0.70] ); ( r_{GG} \in [0.02, 0.16] )</td>
</tr>
<tr>
<td><img src="image1.png" alt="Map/Region" /></td>
<td><img src="image2.png" alt="Structure" /></td>
</tr>
</tbody>
</table>

| \( N_0 = 2 \) | 15%; atom symmetry: \( O_h \), 68%; center symmetry: \( O_h \), 98%; \( r_{GH} \in [0.61, 0.68] \); \( r_{GG} \in [0.16, 0.42] \) |
| ![Map/Region](image3.png) | ![Structure](image4.png) |
51%: atom symmetry $O_h$, 92% $C$; center symmetry $T_d$, 69% $T$; $r_{GH} \in [0.67, 0.71]$; $r_{GG} \in [0.32, 1.6]$

25%: atom symmetry $O_h$, 96% $C$; center symmetry $T_d$, 80% $T$; $r_{GH} \in [0.69, 0.71]$; $r_{GG} \in [2.4, 4]$
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Supplementary Information

Typical Structures of Stable Dimer Trapping Sites: Model II

Typical structures are presented in order of increasing $N_0$, the number of host atoms removed from the crystal. For each $N_0$, the representative site structures are shown with the reference to clustering map discussed in the main text. The area populated by the structures of certain type is given as the percentage of the whole map area. Dominant symmetry of host environment with respect to atom and dimer center (T, O, C for tetrahedral, octahedral, and cuboctahedral, respectively) is provided as established by the radial distribution function analysis (see main text). The ranges of the minimum distances between guest and host atoms $r_{GH}$ and distances between guest atoms $r_{GG}$ are also shown in units of lattice parameter.

In the structure plots, guest atoms are shown in red together with the first coordination polyhedron. Host atoms composing the first coordination polyhedron are shown in blue, the rest — in gray. Arrows at the bottom-left indicate x, y, z ideal lattice vectors of the length $a/2$.

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<thead>
<tr>
<th>map/region</th>
<th>representative structures</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_0 = 0$</td>
<td></td>
</tr>
<tr>
<td>2%; atom symmetry: $T_d, 99% T$; center symmetry: $T_d, 100% T$; $r_{GH} \in [0.40, 0.42]$; $r_{GG} \in [0.02, 0.28]$</td>
<td><img src="image" alt="1(a)" /></td>
</tr>
<tr>
<td>2%; atom symmetry: $T_d, 98% T$; center symmetry: $T_d, 65% T$; $r_{GH} \in [0.42, 0.44]$; $r_{GG} \in [0.45, 0.92] \cup [1.06, 1.31] \cup [1.46, 2.23]$</td>
<td><img src="image" alt="1(b)" /></td>
</tr>
<tr>
<td>6%; atom symmetry: $O_h, 91% O$; center symmetry: $O_h, 93% O$; $r_{GH} \in [0.42, 0.47]$; $r_{GG} \in [0.02, 0.28]$</td>
<td>![image]</td>
</tr>
</tbody>
</table>
\[2\%: \text{atom symmetry:} O_h, 94\%; \text{center symmetry:} T_d, 61\%; r_{GH} \in [0.47, 0.56]; r_{GG} \in [0.28, 0.45]\]

\[18\%: \text{atom symmetry:} O_h, 94\%; \text{center symmetry:} T_d, 79\%; r_{GH} \in [0.47, 0.56]; r_{GG} \in [0.02, 0.28] \cup [0.45, 0.79] \cup [0.92, 1.06] \cup [1.16, 1.46] \cup [1.53, 1.75]\]

\[N_0 = 1\]

\[10\%: \text{atom symmetry:} O_h, 38\%; \text{center symmetry:} O_h, 90\%; r_{GH} \in [0.51, 0.63] \cup [0.72, 0.84]; r_{GG} \in [0.31, 0.60] \cup [0.75, 1.05]\]
$N_0 = 2$

17%; atom symmetry: $O_h$, 93%; center symmetry: $T_d$, 84%; $r_{GH} \in [0.62, 0.76]$; $r_{GG} \in [0.56, 0.61] \cup [0.63, 0.8] \cup [1.79, 2.27]$

$N_0 = 7$

9%; atom symmetry: $T_d$, 94%; center symmetry: $T_d$, 73%; $r_{GH} \in [0.80, 0.97]$; $r_{GG} \in [0.83, 1.05]$
\( N_0 = 8 \)

9\%, atom symmetry: \( T_d, 97\% T \), center symmetry: \( T_d, 79\% T \), \( r_{GH} \in [0.82, 0.97] \); \( r_{GG} \in [1.05, 1.26] \cup [1.55, 1.82] \)

\( N_0 = 10, 11 \)

7\%, atom symmetry: \( O_h, 68\% O \), center symmetry: \( T_d, 83\% T \), \( r_{GH} \in [0.90, 1.07] \); \( r_{GG} \in [1.07, 1.8] \)

\( N_0 = 12 \)

3\%, atom symmetry: \( O_h, 89\% O \), center symmetry: \( T_d, 68\% T \), \( r_{GH} \in [0.92, 1.07] \); \( r_{GG} \in [1.17, 1.64] \)