Configurations of the third nearest-neighbor molecules forming a vacancy wall and an addition of a CO$_2$ molecule in the vacancy of solid CO$_2$ at $T = 0, 100, \text{and } 200 \text{ K}$ studied by Monte Carlo simulation technique

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Abstract

Configurations of the molecules on the wall of a vacancy, formed by removing a central and its first and second nearest-neighbor (NN) molecules in solid CO$_2$ with the $Pa\bar{3}$ structure, were calculated by the Monte Carlo simulation technique at $T = 0, 100, \text{and } 200 \text{ K and a nominal pressure of } P = 1 \text{ bar. It was found that the average deviations of both the center-of-mass and the orientational coordinates of the molecules from the unperturbed coordinates had a three-fold symmetry about a body diagonal axis of the vacancy. It was also found that a single CO$_2$ molecule, initially placed in the center of the vacancy, was stabilized at a position close to one of the 12 first-NN sites with the corresponding orientation. This paper is a continuation of arXiv:1711.04976 [cond-mat.mtrl-sci] (2017) and arXiv:1809.04291 [cond-mat.mtrl-sci] (2018).}

Key words: Monte Carlo simulation, solid CO$_2$, vacancy, finite temperatures

1. Introduction

The present work is a continuation of the precedent two papers$^{1,2}$ that investigated molecular configurations surrounding a single vacancy in solid CO$_2$ with the $Pa\bar{3}$ structure$^{3,4}$ at temperatures of $T = 0, 100, \text{and } 200 \text{ K using the Monte Carlo (MC) simulation technique}$ and a Kihara core potential model.$^6$ In those papers, the basic cell was cubic, and contained 2047 (=2048-1) molecules, in which the periodic
boundary condition was applied. It was found that at $T = 0$ and 100 K, the orientational changes were greater for the three nearest-neighbor (NN) molecules and the equivalent three other molecules located in close proximity to the positions of the oxygen atoms associated with a CO$_2$ molecule that had been removed to make a vacancy at the origin. By contrast, such changes disappeared at $T = 200$ K as the molecular orientations were randomized due to high temperature. In the first part of the present work, the vacancy was made larger by removing a molecule in the center and its first and second NN molecules: namely, 19 molecules were removed to make a cubic vacancy. Hence, the third NNs consisting of 24 molecules form a wall of the vacancy, and these molecules will be hereafter referred to as “wall molecules”. Thus, the total number of molecules in the cubic basic cell with the vacancy was 2029 ($=2048-19$). For reference, simulations were also done for the CO$_2$ crystal without vacancy. In the second part of the present work, a stable configuration of a CO$_2$ molecule that was initially placed at the origin of the vacancy was studied. Since solid CO$_2$ sublimes at $T = 194.7$ K at the ambient pressure, one may expect that the CO$_2$ molecule moves freely in the vacancy. The present simulations showed, however, that the CO$_2$ molecule stayed close to one of the 12 first NN sites in the vacancy. The major interest of the present work is to see the influence of temperature on the configurations of the 24 wall molecules and the CO$_2$ molecule added in the vacancy.

2. Computational procedure

The computational procedure was similar to those used in Refs. 1 and 2. The lattice constants $a$ used at different temperatures were assumed in reference to experiments$^{2,7}$ as follows: $a = 5.53725 + 4.679 \times 10^{-6} T^2$ in units of Å. The edge of the cubic basic cell consisted of eight primitive unit cells so that the length was 44.3 Å at $T = 0$ K. Note, therefore, that the vacancies form a cubic lattice with a lattice constant of 44.3 Å that is far enough for vacancies to interact with each other because the maximum interaction range between molecules was set to be 15 Å in the present simulation. The same applies to the cases of $T = 100$ and 200 K. The periodic boundary condition was applied to the cubic basic cell. The pressure was not calculated but likely to be ambient as the temperature dependence of $a$ was determined from the experiments at ambient pressure as described above. In the first part of the present work, there were 2029 molecules in the cubic basic cell containing a cubic vacancy that was formed by removing 19 molecules. The initial crystal structure was $Pa3$, and both the center-of-mass (CM) and orientational coordinates of all molecules in the cubic basic
cell were randomized within a range of \( -0.2 \, \text{Å} < \Delta x, \Delta y, \Delta z < 0.2 \, \text{Å} \) (1 Å = 0.1 nm) for CM positions and within a range of \(-30^\circ < \Delta \theta, \Delta \phi < 30^\circ\) for molecular orientations. These are collectively expressed as \( \{\Delta r, \Delta \psi\} = \{0.2 \, \text{Å}, 30^\circ\} \), hereafter. The randomized structure returned to a structure close to \( Pa3 \) in the next computational job as indicated by the CM positions, the molecular orientations as well as the total crystal energy. The values of \( \{\Delta r, \Delta \psi\} \) were decreased stepwise to \( \{0.1 \, \text{Å}, 10^\circ\} \) in the default cases. The last 40 data were chosen for analysis after the total energy had been stable. A single computational job contained 100,000 rounds of molecular energy calculations over all molecules in a random order. The acceptance ratio was only \( 5 \times 10^{-3} \% \). The major reason for the extremely low acceptance ratio is attributable to the large values for \( \{\Delta r, \Delta \psi\} \) as new molecular configurations are mostly rejected, but the actual reason is still under investigation. The computations were done on regular desktop computers using gfortran, a Linux Fortran. Each job took about 130 minutes. The total energy of the \( \text{CO}_2 \) crystal reached the equilibrium approximately after about 20 jobs from the start. In the second part of the present work, a \( \text{CO}_2 \) molecule oriented in the (111)-direction was initially placed at the origin of the vacancy, and the MC simulations were performed at the three different temperatures to determine the stable CM position and the orientation of the molecule. Note that solid \( \text{CO}_2 \) (dry ice) sublimes at 194.7 K at ambient pressure, while solid \( \text{CO}_2 \) at 200 K was simulated in the present work. This does not seem to alter the major results in the present work as the potential model used does not have such a high accuracy as to quantitatively reproduce the sublimation temperature though it needs to be proved. It should be noted that unlike regular MC simulations, the energy calculations in the present work, and in Refs. 1 and 2 as well, were carried out not by randomly choosing a molecule in the cubic basic cell in every calculation but in a random sequence over all molecule in the cubic basic cell in each calculation. This protocol seems to be most efficient for the crystal energy conversion, but the ergodicity of the protocol needs to be proved.

3. Results and Discussion

3.1 Wall molecules in the vacancy

Figure 1 shows the configurations of the wall molecules at \( T = 0 \, \text{K} \) (after simulation) observed from the [111] direction of the \( Pa3 \) crystal. The molecules are numbered from 1 to 24. Each molecule is closely located on an \( fcc \) lattice site, and closely oriented along one of the body diagonals of the cubic lattice.
brown sphere and two red spheres in a molecule indicate carbon and oxygen atoms, respectively, with
the van der Waals radii.

Table 1 shows the calculated data at \( T = 200 \) K for explaining the major results of the present work. In
the table, the meanings of the notations are as follows:

- **Mol. No.**: molecular label shown in Fig. 1,
- **Position**: approximate direction of the molecule seen from the origin of the vacancy,
- **Orientation**: orientation of the molecule in the \( Pa3 \) structure,
- \( \delta x, \delta y, \) and \( \delta z \): CM deviations in the \( x-, y-, \) and \( z\)-directions in units of Å from the initial positions of the
  \( Pa3 \) structure with the vacancy, respectively,
- \( \delta p, \delta q, \) and \( \delta r \): deviations of the unit vector along the molecular axis in the \( x-, y-, \) and \( z\)-directions in
  units of Å from the initial orientation of the \( Pa3 \) structure with the vacancy, respectively, and
- \( \delta E \): molecular energy in units of K (1 K = \( 1.38054 \times 10^{-23} \) J) measured from the molecular energy in
  the unperturbed crystal structure with the vacancy.

Note in Fig. 1 that there are three molecules forming a triangle at each corner of the cubic vacancy, and
in Table 1, the three molecules are shown in different colors. In Table 1, it is seen that the CM and
orientational deviations, \{\( \delta x, \delta y, \delta z \)\} and \{\( \delta p, \delta q, \delta r \)\}, respectively, have a three-fold symmetry about the
[111] direction of the crystal: the combinations are 2-5-13, 4-11-14, 6-10-17, 7-16-20, 8-15-19, and 12-18-21 in terms of Molecular Number (Label). In each of the combinations, the molecular energies \( \delta E \) are also very close. The three-fold symmetry was also present for \( T = 0 \) and 100 K cases.

Table 2 shows average deviations of the CM positions, \( \langle r \rangle \), the orientations, \( \langle \Omega \rangle \); average standard
deviations (STDVs) of the CM positions, \( \langle \langle r \rangle \rangle \), and the orientations, \( \langle \langle \Omega \rangle \rangle \), over the wall molecules at
different temperatures in reference to the CM positions and the orientations in the \( Pa3 \) structure with the
vacancy at the corresponding temperature. Note that \( \langle r \rangle \) and \( \langle \Omega \rangle \) are the absolute values. The results in
Table 2 are to be compared with those of a CO\(_2\) crystal without vacancy, shown in Table 3. It is obvious that
both deviations and STDVs are greater for the wall molecules in the vacancy than for the molecules in perfect
crystal. Since the wall molecules have spaces on one side, all values of \( \langle r \rangle, \langle \Omega \rangle, \langle \langle r \rangle \rangle \) and \( \langle \langle \Omega \rangle \rangle \) in
Table 2 are greater than those in Table 3. The results in Table 2 indicate that the cubic vacancy surrounded
by the wall molecules is quite robust even at high temperature in the sense that the wall molecules change the CM positions only slightly even at $T = 200$ K.

3.2 A single molecule in the vacancy

Figure 2 shows the configurations of the wall molecules and the single molecule (in blue) added in the vacancy at $T = 200$ K, observed from the [111] direction of the $Pa3$ crystal. The single molecule was initially placed at the origin of the cubic vacancy with the (111) orientation, but after the simulation was over, it moved to a position close to the molecular clusters 5-6-11 (in the <1-11> direction from the origin) and 7-8-12 (in the <1-1-1> direction from the origin). The molecule was located close to the position of the first NN molecule that was in the <1-10> direction from the origin, its orientation was approximately (1-1-1), and corresponded to molecule 226 in Ref. 1 in terms of the CM position and the molecular orientation.

Table 4 shows the deviations of CMs, orientations, and molecular energies of the wall molecules at $T = 200$ K. The notations are the same as in Table 1. Unlike in Table 1, the three-fold symmetry is not observed among the wall molecules, most likely because of the presence of the CO$_2$ molecule added in the vacancy. It should be noted that the energy deviations, $\delta E$, are more negative than the counterparts of Table 1 because of the interactions with the CO$_2$ molecule. Since the CO$_2$ molecule is located closer to the molecular clusters 5-6-11 and 7-8-12, the molecular energies of molecules 5, 8, 11, and 12 are significantly lower than those of other wall molecules.

Table 5 shows the average deviations of the CM positions, $\langle r \rangle$, the orientations, $\langle \Omega \rangle$; average STDVs of the CM positions, $\langle\langle r \rangle\rangle$, and the orientations, $\langle\langle \Omega \rangle\rangle$, over the wall molecules forming a vacancy with a single CO$_2$ molecule. The all values tend to increase at higher temperature, but the changes are similar to those in Table 2.

Table 6 shows the average STDVs of the CM positions, $\langle\langle r \rangle\rangle$, and the orientations, $\langle\langle \Omega \rangle\rangle$, of the CO$_2$ molecule added in the vacancy. All values tend to increase at higher temperature, and the changes are more strongly dependent on temperature than those of the wall molecules presumably because the CO$_2$ molecule added in the vacancy is less constrained than the wall molecules.
4. Conclusion

In the first part of the present work, it was found that the average molecular configurations of the wall molecules comprising the vacancy have a three-fold symmetry about a [111] body-diagonal axis of the vacancy. The cubic vacancy structure was maintained even at $T = 200$ K, and both the deviations and the STDVs of the CMs and molecular orientations for the wall molecules were small. This indicates that the cubic vacancy is quite robust to temperature. In the second part of the present work, it was found that a CO$_2$ molecule added to the vacancy stayed in one of the first NN sites with the corresponding orientation. In summarizing the present and the past two papers$^{1,2}$ on classical MC simulations of a molecular solid (maximum 2048 molecules in solid CO$_2$), the following technical results and issues have been made clear:

(i) The crystal energy converged within approximately 100 jobs, each job performing 100,000 molecular energy calculations over all molecules, and taking about 130 minutes, so that the computations were tractable with regular desktop PCs.

(ii) The lattice constants at different temperatures were assumed from experiment in the present and past two papers.$^{1,2}$ For theoretically consistent calculations, the MC simulations must be done using the pressure-constant algorism, which will be studied in the future.

(iii) The acceptance ratio was extremely small, and depended on the values of $\{\Delta r, \Delta \psi\}$: the acceptance ration was higher as the values of $\{\Delta r, \Delta \psi\}$ were set smaller. For MC simulations of molecular fluids, $\{\Delta r, \Delta \psi\}$ are set empirically so that the acceptance ratio becomes $\sim 50\%$. For MC simulations of molecular solids, a good reasoning is required to determine the most appropriate values for $\{\Delta r, \Delta \psi\}$.

(iv) The protocol for simulation used in the present and precedent two papers$^{1,2}$ were different from the standard one,$^5$ and created by intuition because no articles was found on such a protocol. The protocol seemed to be efficient for the crystal energy conversion in molecular solids, but the ergodicity of the protocol needs to be proved.

Acknowledgement

Figures 1 and 2 are depicted using an open software, VESTA, published in: K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data," J. Appl. Crystallogr. 44, 1272 (2011).
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| Mol. No. | Position | Orientation | $\delta x$ (Å) | $\delta y$ (Å) | $\delta z$ (Å) | $\delta p$ | $\delta q$ | $\delta r$ | $\delta E$ (K) |
|--------|----------|-------------|----------------|----------------|----------------|-----------|-----------|-----------|-------------|
| 1      | <111>   | (-111)      | 0.23           | 0.11           | 0.20           | -0.08     | -0.08     | -0.02     | 69.17       |
| 2      | <11-1>  | (-111)      | 0.14           | 0.19           | -0.16          | 0.00      | 0.07      | -0.08     | 84.10       |
| 3      | <111>   | (11-1)      | 0.13           | 0.18           | 0.21           | -0.07     | -0.02     | -0.08     | 69.76       |
| 4      | <11-1>  | (11-1)      | 0.13           | 0.18           | -0.11          | 0.01      | -0.01     | -0.01     | 131.97      |
| 5      | <1-11>  | (11-1)      | 0.21           | -0.18          | 0.12           | 0.07      | -0.07     | 0.01      | 86.90       |
| 6      | <1-11>  | (-111)      | 0.14           | -0.14          | 0.23           | 0.04      | 0.00      | 0.04      | 32.41       |
| 7      | <1-1-1> | (-111)      | 0.11           | -0.14          | -0.19          | -0.01     | 0.01      | -0.02     | 127.01      |
| 8      | <1-1-1> | (11-1)      | 0.12           | -0.25          | -0.16          | 0.00      | 0.04      | 0.04      | 24.94       |
| 9      | <111>   | (1-11)      | 0.22           | 0.21           | 0.13           | -0.01     | -0.07     | -0.08     | 77.14       |
| 10     | <11-1>  | (1-11)      | 0.24           | 0.14           | -0.12          | 0.04      | 0.04      | -0.01     | 40.08       |
| 11     | <1-11>  | (1-11)      | 0.19           | -0.09          | 0.13           | -0.02     | -0.01     | 0.01      | 153.02      |
| 12     | <1-1-1> | (1-11)      | 0.16           | -0.15          | -0.22          | -0.08     | 0.00      | 0.07      | 79.47       |
| 13     | <1-11>  | (1-11)      | -0.18          | 0.13           | 0.19           | -0.08     | 0.00      | 0.07      | 77.03       |
| 14     | <1-11>  | (-111)      | -0.14          | 0.12           | 0.15           | 0.00      | 0.00      | 0.00      | 150.07      |
| 15     | <1-1-1> | (-111)      | -0.12          | 0.16           | -0.22          | 0.04      | 0.00      | 0.04      | 34.12       |
| 16     | <1-1-1> | (1-11)      | -0.18          | 0.11           | -0.12          | -0.01     | 0.01      | 0.02      | 139.45      |
| 17     | <1-11>  | (1-11)      | -0.15          | 0.23           | 0.14           | 0.01      | 0.04      | 0.05      | 34.22       |
| 18     | <1-1-1> | (11-1)      | -0.20          | 0.18           | -0.13          | 0.07      | -0.08     | 0.00      | 90.60       |
| 19     | <1-11>  | (11-1)      | -0.23          | -0.14          | 0.13           | 0.05      | 0.05      | 0.00      | 24.28       |
| 20     | <1-11>  | (11-1)      | -0.12          | -0.17          | 0.10           | 0.01      | -0.01     | 0.01      | 138.16      |
| 21     | <1-11>  | (-111)      | -0.13          | -0.20          | 0.17           | 0.01      | 0.07      | -0.07     | 81.96       |
| 22     | <1-1-1> | (-111)      | -0.21          | -0.12          | -0.18          | -0.07     | -0.08     | -0.01     | 73.48       |
| 23     | <1-1-1> | (11-1)      | -0.19          | -0.22          | -0.08          | -0.02     | -0.08     | -0.07     | 55.90       |
| 24     | <1-1-1> | (11-1)      | -0.11          | -0.20          | -0.20          | -0.08     | -0.01     | -0.08     | 66.58       |
Table 2. Average deviations of the CM positions, $<r>$, and the orientations, $<\Omega>$; average STDVs of the CM positions, $<<r>>$, and the orientations, $<<\Omega>>$, over all the wall molecules.

| Temp. (K) | Deviation | STDV       |
|-----------|-----------|------------|
|           | $<r>$     | $<\Omega>$ | $<<r>>$   | $<<\Omega>>$ |
| 0         | 0.1       | 4.1        | 0.03      | 1.2          |
| 100       | 0.1       | 3.9        | 0.03      | 1.1          |
| 200       | 0.3       | 4.9        | 0.04      | 1.4          |

Table 3. Average deviations of the CM positions, $<r>$, and the orientations, $<\Omega>$; average STDVs of the CM positions, $<<r>>$, and the orientations, $<<\Omega>>$, for molecules in perfect crystal.

| Temp. (K) | Deviation | STDV       |
|-----------|-----------|------------|
|           | $<r>$     | $<\Omega>$ | $<<r>>$   | $<<\Omega>>$ |
| 0         | 0.0       | 1.8        | 0.02      | 0.8          |
| 100       | 0.0       | 1.6        | 0.02      | 0.8          |
| 200       | 0.0       | 2.0        | 0.03      | 1.0          |
Table 4. Deviations of CMs, orientations, and molecular energies of the wall molecules forming a vacancy with a single molecule at \( T = 200 \) K. The notations are the same as in Table 1.

| Mol. No. | Position | Orientation | \( \delta_x \) (Å) | \( \delta_y \) (Å) | \( \delta_z \) (Å) | \( \delta p \) | \( \delta q \) | \( \delta r \) | \( \delta E \) (K) |
|----------|----------|-------------|------------------|------------------|------------------|-------------|-------------|-------------|---------------|
| 1        | <111>    | (-111)      | -0.09            | -0.11            | -0.16            | -0.05       | -0.06       | 0.01        | -238.12       |
| 2        | <11-1>   | (-111)      | -0.14            | -0.09            | 0.12             | -0.03       | 0.03        | -0.06       | -238.93       |
| 3        | <111>    | (11-1)      | -0.13            | -0.14            | -0.07            | -0.05       | 0.01        | -0.04       | -236.33       |
| 4        | <11-1>   | (11-1)      | -0.13            | -0.14            | 0.08             | 0.02        | -0.03       | -0.01       | -115.73       |
| 5        | <1-11>   | (11-1)      | -0.08            | 0.07             | -0.07            | 0.04        | -0.08       | -0.03       | -678.72       |
| 6        | <1-1>    | (11-1)      | -0.13            | 0.08             | -0.17            | 0.06        | 0.03        | 0.03        | -377.19       |
| 7        | <1-1-1>  | (-111)      | -0.09            | 0.10             | 0.16             | 0.01        | 0.01        | 0.00        | -201.10       |
| 8        | <1-1-1>  | (11-1)      | -0.06            | 0.16             | 0.08             | 0.04        | -0.04       | 0.00        | -595.28       |
| 9        | <111>    | (1-11)      | -0.16            | -0.06            | -0.11            | 0.00        | -0.05       | -0.05       | -220.96       |
| 10       | <11-1>   | (1-11)      | -0.16            | -0.11            | 0.07             | 0.02        | 0.06        | 0.03        | -220.56       |
| 11       | <1-11>   | (1-11)      | -0.17            | 0.04             | -0.12            | -0.01       | 0.03        | 0.03        | -550.05       |
| 12       | <1-1-1>  | (1-11)      | -0.13            | 0.09             | 0.08             | -0.04       | -0.04       | 0.00        | -635.49       |
| 13       | <1-11>   | (1-11)      | 0.11             | -0.11            | -0.09            | -0.07       | -0.03       | 0.03        | -237.49       |
| 14       | <1-11>   | (-111)      | 0.07             | -0.11            | -0.17            | -0.01       | -0.02       | -0.03       | -104.10       |
| 15       | <11-1>   | (-111)      | 0.09             | -0.09            | 0.14             | 0.06        | 0.03        | 0.02        | -216.91       |
| 16       | <11-1>   | (1-11)      | 0.13             | -0.09            | 0.10             | -0.03       | -0.01       | 0.03        | -118.77       |
| 17       | <1-11>   | (11-1)      | 0.04             | -0.11            | -0.13            | 0.03        | 0.03        | 0.06        | -219.45       |
| 18       | <11-1>   | (11-1)      | 0.05             | -0.13            | 0.10             | 0.02        | -0.06       | -0.03       | -237.84       |
| 19       | <1-1-1>  | (11-1)      | 0.12             | 0.11             | -0.09            | 0.02        | 0.06        | 0.03        | -224.36       |
| 20       | <1-11>   | (11-1)      | 0.11             | 0.15             | -0.09            | 0.03        | -0.04       | -0.01       | -151.31       |
| 21       | <1-11>   | (-111)      | 0.11             | 0.08             | -0.14            | -0.04       | 0.02        | -0.06       | -248.19       |
| 22       | <1-1-1>  | (-111)      | 0.03             | 0.11             | 0.16             | -0.04       | -0.05       | 0.01        | -228.59       |
| 23       | <1-1-1>  | (11-1)      | 0.12             | 0.07             | 0.12             | 0.01        | -0.04       | -0.06       | -248.59       |
| 24       | <1-1-1>  | (11-1)      | 0.08             | 0.16             | 0.09             | -0.05       | 0.01        | -0.04       | -248.31       |
Table 5. Average deviations of the CM positions, <\textit{r}>, the orientations, <\textit{\Omega}>; average STDVs of the CM positions, <<\textit{r>>>, and the orientations, <<\textit{\Omega>>>, over the wall molecules forming a vacancy that includes a CO\textsubscript{2} molecule (shown in blue in Fig. 2) in the vacancy.

| Temp. (K) | Deviation | STDV |
|-----------|-----------|------|
|           | <\textit{r}> | <\textit{\Omega}> | <<\textit{r>>> | <<\textit{\Omega>>> |
|          | (Å)       | (deg.) | (Å) | (deg.) |
| 0        | 0.1       | 3.9    | 0.02 | 0.6 |
| 100      | 0.2       | 4.1    | 0.03 | 1.1 |
| 200      | 0.2       | 4.1    | 0.03 | 1.1 |

Table 6. Average STDVs of the CM position, <<\textit{r>>>, and the orientation, <<\textit{\Omega>>>, of the CO\textsubscript{2} molecule (shown in blue in Fig. 2) added in the vacancy.

| Temp. (K) | STDV |
|-----------|------|
|           | <<\textit{r>>> | <<\textit{\Omega>>> |
|          | (Å) | (deg.) |
| 0        | 0.02 | 0.7 |
| 100      | 0.03 | 1.1 |
| 200      | 0.05 | 1.7 |
Figure captions

Fig. 1. Configurations of the wall molecules at $T = 0$ K observed from the [111] direction of the Pa3 crystal.

Fig. 2. Configurations of the wall molecules and the CO$_2$ molecule (in blue) added in the cubic vacancy at $T = 200$ K observed from the [111] direction of the Pa3 crystal.
Fig. 1. Configurations of the wall molecules at $T = 0$ K observed from the [111] direction of the $Pa\overline{3}$ crystal.
Fig. 2. Configurations of the wall molecules and the CO$_2$ molecule (in blue) added in the cubic vacancy at $T = 200$ K observed from the [111] direction of the $Pa\bar{3}$ crystal.