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Cite as: AIP Advances 9, 115118 (2019); https://doi.org/10.1063/1.5110322
Submitted: 16 May 2019 . Accepted: 05 November 2019 . Published Online: 22 November 2019

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ABSTRACT
Using a first-principles density functional theory method, we calculated the vibrational spectrum of ice XIII. In combination with spectroscopic experiments, we demonstrated that the two characteristic hydrogen bond (H-bond) peaks in the translational region of ice V (the hydrogen-disordered counterpart of ice XIII) recorded by inelastic neutron scattering originate from two basic H-bond vibrational modes. We first observed this phenomenon when studying ice Ic and then confirmed it when studying ice XIV, XVI, and XVII. This study of high-pressure ice XIII supports our theory that two basic H-bond modes exist as a general rule among the ice family. The "isolated O–H vibration modes" found by Whale et al. when studying ice XV are also discussed in this work.

I. INTRODUCTION
Despite its simplicity, ice has more than 18 crystalline phases under different pressures and temperatures. Among the crystalline phases of ice, ice XIII is the hydrogen-ordered counterpart of ice V and crystallizes in the space group \( P2_1/a \). Ice XIII was discovered in 2006 by Salzmann et al., who found that ice XIII formed upon cooling ice V doped with hydrochloric acid. Since the electron density has a large distribution in the ice lattice, we chose to use generalized gradient approximation (GGA) in this work. To test the exchange–correlation functionals, we employed RPBE, PBE, PW91, WC, and PBESOL for geometry optimization, resulting in densities of 1.13, 1.30, 1.31, 1.44, and 1.45 g/cm\(^3\), respectively. Thus, the RPBE functional produced the most similar structure to the experimental one. Because the length of the intermolecular H-bond is related to density and the vibrational frequency is highly sensitive to

II. COMPUTATIONAL METHOD
First-principles density functional theory (DFT) implemented in the CASTEP code was used to perform geometric optimization and phonon calculations on the structure of ice XIII. The primitive cell of ice XIII was constructed according to Salzmann’s report in 2006, and its density was 1.06 g/cm\(^3\). Since the electron density has a large distribution in the ice lattice, we chose to use generalized gradient approximation (GGA) in this work. To test the exchange–correlation functionals, we employed RPBE, PBE, PW91, WC, and PBESOL for geometry optimization, resulting in densities of 1.13, 1.30, 1.31, 1.44, and 1.45 g/cm\(^3\), respectively. Thus, the RPBE functional produced the most similar structure to the experimental one. Because the length of the intermolecular H-bond is related to density and the vibrational frequency is highly sensitive to
H-bond length, the best functional for this ice phase was determined to be RPBE. The energy and self-consistent field tolerances were set as $1 \times 10^{-9}$ eV/atom for phonon calculation. The energy cutoff was 830 eV, and the K-point grid was $2 \times 2 \times 1$. Norm-conserving pseudopotential was used to calculate the PDOS and polarizability. The Raman spectrum could be plotted directly by CASTEP analysis, and the IR spectrum was derived from vibrational analysis. Since the RPBE functional underestimates the intermolecular forces, the hydrostatic pressure was set as 1.0 GPa; this provided a better fit to the experimental data compared to 0.5 GPa, which was used in Ref. 13.

III. RESULTS AND DISCUSSION

The simulated Raman, IR, and PDOS spectra are shown in four parts in Fig. 1. Because of the large ranges of Raman and IR spectral intensities, the relative proportions of the three types of spectra were adjusted to allow for comparison. A primitive cell with 28 molecules has $28 \times 3 \times 3 = 249$ optic normal modes. Since inelastic neutron scattering (INS) collects phonon signals throughout the Brillouin zone (BZ), there are qualitative similarities between the INS and PDOS spectra. Table I presents the main peaks of PDOS together with the INS data in the first two columns. According to our experience, the hydrogen-ordered counterpart of the ice phase presents sharper peaks than the hydrogen-disordered phase. Herein, we take the INS data of ice V as those of ice XIII because no such data have been reported until now. The Raman-active normal vibration frequencies at the BZ center are listed in the third column of Table I, and the corresponding intensities are listed in the fourth column. Given the lack of experimental IR data, the Raman results in the last column of Table I are presented only for comparison. Some representative peaks are discussed in detail, and the dynamic processes are described in the supplementary material.

In the intermolecular translation band, there are 81 normal modes ranging from 50 to 318 cm$^{-1}$ in the 28-molecule primitive cell. In this region, the vibrational modes of molecules are all translational motions. Obviously, it is difficult to analyze the vibrational modes individually. However, we found a clue in the simplest model of hydrogen-ordered ice, Ic (see Ref. 19), which contains two molecules in one primitive cell. In this model, there are only two kinds of H-bond vibration modes. According to the Bernal–Fowler rules, each water molecule is connected to four neighbors by H-bonds to form a tetrahedral structure in the ice crystal. In the strong vibration mode, the central molecule vibrates along the HOH angle bisector with the four H-bonds oscillating at the same time. In the other two degenerate modes, the central molecule vibrates along two H-bonds, while the other two H-bonds remain unchanged. In the Ic model of ice, the strength ratio between the two vibrational modes is $\sqrt{2}$. These two modes contribute to the two main H-bond peaks in the translation band. In our previous investigations, we also observed this phenomenon in ice XIV, XVI, and XVII. In this work, the two basic vibration modes of ice XIII are discussed. To analyze the vibrational direction of the H-bond modes, we treated the motion of oxygen as that of the molecular mass center and took the molecule with the largest amplitude as representative of a primitive cell. Since the vibrational modes of molecules are translational motions in this region, we considered the motion of oxygen to be the motion of the molecule. To analyze the distributions of the two kinds of translation modes using our self-compiled program, the mode types were distinguished based on the vibrational direction of oxygen. Although the local structure retained a tetrahedral geometry under pressure, significant deformation from the ideal model was observed in Ic. Therefore, both strong and weak H-bond modes were distributed in the structure, with the vibrational direction of oxygen close to the angle bisector below 45° corresponding to the strong mode and vice versa (the source code is provided as a supplementary material S1). A diagram of the analysis is shown in Fig. 2. In Fig. 2, the modes above 280 cm$^{-1}$ are the strong modes, while those below 280 cm$^{-1}$ are the weak modes. The overlap between 260 and 280 cm$^{-1}$ is a result of the distribution of both kinds.

![FIG. 1. Computed Raman, IR, and PDOS spectra of ice XIII presented in the regions of the four vibrational bands: (a) intermolecular translation band, (b) intermolecular libration band, (c) intramolecular bending band, and (d) intramolecular stretching band.](image-url)
TABLE I. Comparison of the computational results and experimental data. The main PDOS peaks are compared with the INS data. The frequencies of the Raman-active normal modes are compared with the experimental Raman peaks.

| PDOS | Neutr. scattering (Ref. 32) | Normal modes (Raman active) | Raman intensity (Refs. 13/33) | Raman scattering (Refs. 13/33) |
|------|----------------------------|-----------------------------|-------------------------------|-------------------------------|
| 50   | 0.02                       |                              |                               |                               |
| 68   | 0.15                       |                              |                               |                               |
| 78   | 0.64                       | 78                           | 0.05                          |                               |
| 80   | 0.33                       | 82                           | 0.13                          |                               |
| 87   | 0.02                       | 90                           | 0.24                          |                               |
| 90   | 0.10                       | 95                           | 0.11                          |                               |
| 96   | 0.03                       | 98                           | 0.32                          |                               |
| 108  | 0.18                       | 115                          | 0.18                          |                               |
| 115  | 0.08                       | 118                          | 0.08                          |                               |
| 123  | 0.08                       | 127                          | 0.49                          |                               |
| 127  | 0.49                       | 130                          | 0.01                          |                               |
| 130  | 0.01                       | 134                          | 0.08                          |                               |
| 134  | 0.08                       | 143                          | 0.62                          |                               |
| 143  | 0.62                       | 154                          | 0.91                          |                               |
| 154  | 0.91                       | 155                          | 0.61                          |                               |
| 155  | 0.61                       | 164                          | 1.01                          |                               |
| 167  | 3.63                       | 169                          |                               |                               |
| 169  |                               | 172                          | 0.55                          |                               |
| 172  |                               | 173                          | 0.55                          |                               |
| 173  |                               | 186                          | 0.61                          |                               |
| 186  | 0.61                       | 189                          | 2.13                          |                               |
| 189  | 2.13                       | 189                          | 1.19                          |                               |
| 189  | 1.19                       | 198                          | 1.59                          |                               |
| 198  | 1.59                       | 199                          | 1.10                          |                               |
| 201  | 1.10                       | 202                          | 0.82                          |                               |
| 202  | 0.82                       | 207                          | 0.53                          |                               |
| 218  | 1.04                       | 223                          | 0.71                          |                               |
| 223  | 0.71                       | 242                          | 0.57                          |                               |
| 242  | 0.57                       | 246                          | 0.08                          |                               |
| 246  | 0.08                       | 261                          | 0.15                          |                               |
| 261  | 0.15                       | 265                          | 0.12                          |                               |
| 265  | 0.12                       | 272                          | 0.91                          |                               |
| 272  | 0.91                       | 273                          | 0.91                          |                               |
| 273  | 0.91                       | 289                          | 0.42                          |                               |
| 289  | 0.42                       | 297                          | 0.40                          |                               |
| 297  | 0.40                       | 315                          | 0.31                          |                               |
| 315  | 0.31                       | 318                          | 0.50                          |                               |
| 318  | 0.50                       | 524                          | 0.45                          |                               |
| 524  | 0.45                       | 532                          | 3.96                          |                               |
| 532  | 3.96                       | 534                          | 1.94                          |                               |
| 534  | 1.94                       | 554                          | 0.20                          |                               |
| 554  | 0.20                       | 559                          | 1.55                          |                               |
| 559  | 1.55                       | 577                          | 4.58                          |                               |
| 577  | 4.58                       | 577                          | 4.58                          |                               |
| 577  | 4.58                       | 579                          | 0.48                          |                               |
| 579  | 0.48                       | 592                          | 4.51                          |                               |
| 592  | 4.51                       | 598                          | 0.17                          |                               |
| 598  | 0.17                       | 608                          | 8.26                          |                               |
| 608  | 8.26                       | 613                          | 8.26                          |                               |
| 613  | 8.26                       | 603                          | 8.26                          |                               |
| PDOS | Neutr. scattering (Ref. 32) | Normal modes (Raman active) | Raman intensity | Raman scattering (Refs. 13/33) |
|------|---------|----------------|-----------------|-----------------|
| 626  | 629     | 620            | 1.92            | 629/-           |
| 633  | 633     | 633            | 2.23            |                 |
| 633  | 633     | 633            | 8.20            |                 |
| 653  | 658     | 652            | 0.17            | 633/2.23        |
| 664  | 664     | 664            | 1.76            |                 |
| 670  | 675     | 672            | 1.02            |                 |
| 686  | 689     | 682            | 0.57            |                 |
| 697  | 697     | 697            | 4.37            | 686/-           |
| 703  | 703     | 703            | 2.56            |                 |
| 707  | 717     | 707            | 3.26            |                 |
| 719  | 719     | 719            | 1.18            |                 |
| 742  | 745     | 742            | 4.80            | 737/-           |
| 747  | 747     | 747            | 1.31            |                 |
| 752  | 752     | 752            | 5.07            |                 |
| 759  | 759     | 759            | 4.04            |                 |
| 764  | 772     | 764            | 2.12            |                 |
| 774  | 774     | 774            | 1.79            |                 |
| 787  | 788     | 781            | 0.33            |                 |
| 802  | 802     | 802            | 1.38            |                 |
| 808  | 808     | 808            | 1.14            |                 |
| 816  | 812     | 818            | 2.55            |                 |
| 834  | 834     | 834            | 1.92            |                 |
| 837  | 837     | 837            | 3.47            |                 |
| 843  | 836     | 849            | 2.38            |                 |
| 868  | 868     | 868            | 1.03            |                 |
| 890  | 897     | 881            | 0.84            |                 |
| 908  | 904     | 904            | 4.77            | 906/-           |
| 926  | 926     | 926            | 5.70            |                 |
| 944  | 947     | 939            | 2.14            |                 |
| 949  | 949     | 949            | 2.24            |                 |
| 980  | 980     | 980            | 3.71            |                 |
| 984  | 991     | 982            | 3.08            |                 |
| 1629 | 1629    | 1629           | 4.74            |                 |
| 1633 | 1633    | 1633           | 2.62            |                 |
| 1634 | 1634    | 1634           | 2.86            |                 |
| 1638 | 1638    | 1638           | 1.16            |                 |
| 1667 | 1667    | 1667           | 3.76            |                 |
| 1669 | 1669    | 1669           | 1.76            |                 |
| 1677 | 1677    | 1677           | 8.20            |                 |
| 1683 | 1683    | 1683           | 5.34            |                 |
| 1691 | 1691    | 1691           | 1.44            |                 |
| 1698 | 1698    | 1695           | 3.61            |                 |
| 1702 | 1702    | 1702           | 10.44           |                 |
| 1714 | 1714    | 1714           | 3.41            |                 |
| 1719 | 1719    | 1719           | 5.67            |                 |
| 1722 | 1721    | 1721           | 1.43            |                 |
| 3199 | 3200    | 3196           | 7972.60         | 3190/3181       |
| 3204 | 3204    | 3204           | 43.18           |                 |
| 3231 | 3231    | 3231           | 71.47           |                 |
| 3240 | 3240    | 3240           | 614.97          |                 |
| 3250 | 3250    | 3250           | 143.47          |                 |
| 3256 | 3256    | 3256           | 525.69          |                 |
| 3262 | 3264    | 3264           | 674.75          |                 |
of modes and system errors due to the difference between the oxygen atom and the mass center. Because clustered vibrational modes and acoustic phonons exist at wavenumbers much lower than 230 cm$^{-1}$, the diagram below 230 cm$^{-1}$ is not discussed herein. In consideration of the summed PDOS, we characterized the two groups of peaks in the translational band as strong H-bonds (above 280 cm$^{-1}$) and weak H-bonds (between 230 and 280 cm$^{-1}$). The peaks at lower wavenumbers can be attributed to clustered molecular vibrations, non-H-bond vibrations, and acoustic vibrations. The three smooth bands can be seen in the INS spectrum of ice V.

Some representative modes are shown in Fig. 3. The normal mode at 318 cm$^{-1}$ corresponds to the vibration of gold molecules along their angle bisector, which is a typical of the strong H-bond mode. The mode at 223 cm$^{-1}$ is created by the vibration of gold molecules along two H-bonds, corresponding to a weak vibrational mode.

Salzmann et al. reported six Raman scattering peaks of ice XIII at 230, 248, 267, 282, 308, and 325 cm$^{-1}$, corresponding to the normal modes at 198, 218, 242, 273, 297, and 318 cm$^{-1}$, respectively. The experimental peak at 169 cm$^{-1}$ may correspond to the normal mode at 167 cm$^{-1}$.

In the intermolecular librational band, there are 84 normal modes ranging from 524 to 987 cm$^{-1}$. There are three kinds of molecular vibration modes: rocking (back-and-forth rotation of the entire molecule around an axis perpendicular to the molecular plane), wagging (back-and-forth rotation of the molecule around an axis in the molecular plane perpendicular to the bisector of the HOH angle), and twisting (back-and-forth rotation around an axis coincident with the HOH angle bisector). Two representative modes are shown in Fig. 3. For the mode at 839 cm$^{-1}$, two gold molecules vibrate in a twisting mode, whereas the other one vibrates in a

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**TABLE I. (Continued.)**

| PDOS | Neutr. scattering (Ref. 32) | Normal modes (Raman active) | Raman intensity (Refs. 13/33) | Raman scattering (Refs. 13/33) |
|------|-----------------------------|-----------------------------|-------------------------------|-------------------------------|
| 3271 | 71.62                       | 3294                        | 1468.70                       | 3297/-                        |
| 3288 | 423.19                      | 3307                        | 1096.55                       | 3314                          |
| 3300 | 3297                        | 3314                        | 837.35                        | 3307/1096.55                  |
| 3320 | 1096.55                     | 3342                        | 764.66                        | 3345/1096.55                  |
| 3346 | 837.35                      | 3365                        | 360.83                        | 3373                          |
| 3387 | 574.38                      | 3393                        | 204.76                        | 3412                          |
| 3417 | 203.61                      | 3415                        | 71.73                         | 3422                          |
| 3414 | 101.80                      | 3424                        | 485.71                        | 3430                          |
| 3439 | 131.59                      | 3431                        | 30.25                         | 3431                          |
| 3440 | 175.88                      | 3441                        | 101.80                        | 3439                          |
| 3441 | 150.24                      |                             |                               | 3441                          |

FIG. 2. Distributions of the strong (green) and weak (blue) H-bond modes of ice XIII in the range of 230–330 cm$^{-1}$. Both types of modes contribute to the sum of PDOS features, as shown in the inset diagram. Note that there is some overlap between modes below 280 cm$^{-1}$.
wagging mode. For the mode at 524 cm\(^{-1}\), the two gold molecules vibrate in a rocking mode.

According to the experimental data, eight vibrational peaks (481, 517, 542, 571, 629, 686, 737, and 906 cm\(^{-1}\)) were identified by Raman scattering.\(^{13}\) The Raman peaks from 481 to 906 cm\(^{-1}\) correspond to the normal modes at 524, 534, 577, 592, 633, 697, 742, and 904 cm\(^{-1}\). The multipeaks in this region are also reflected in Fig. 1. The PDOS peaks show good agreement with the INS spectrum.\(^{32}\)

In the intramolecular bending band, there are 28 normal modes ranging from 1624 to 1730 cm\(^{-1}\). The vibrational energy of the primitive cell collective mode increases from in-phase vibration to out-of-phase vibration. This trend is shown in the two examples at 1634 and 1730 cm\(^{-1}\) in Fig. 4. In agreement with our previous work,

**FIG. 3.** Examples of four intermolecular vibrational modes at 839, 524, 318, and 223 cm\(^{-1}\). The green arrows represent the vibration direction proportional to the amplitude. The main vibration molecules are shown in gold.

**FIG. 4.** Examples of four representative intramolecular vibrational modes at 3424, 3196, 1730, and 1634 cm\(^{-1}\).
neither Raman nor IR experiments resulted in detectable peaks in this region, possibly because of the large intensity ratios between bending and stretching. For example, the intensity of the Raman peak at 3196 cm$^{-1}$ was 7972.60, whereas the largest intensity of the bending mode was only 10.44 (Table I). In the PDOS spectrum, the peak at 1698 cm$^{-1}$ agrees well with the peak of ice V at 1698 cm$^{-1}$. This is in agreement with our experience that the vibrational frequencies of bending modes remain unchanged under different pressures.

In the intramolecular O–H stretching region, there are 56 normal modes ranging from 3196 to 3446 cm$^{-1}$. These normal modes include two kinds of molecular vibrational modes: symmetric and asymmetric stretching. As shown in Fig. 4, the normal mode at 3196 cm$^{-1}$ corresponds to the symmetric stretching of two gold molecules, whereas the mode at 3424 cm$^{-1}$ indicates that most molecules vibrate through asymmetric stretching. These results agree with the findings of previous studies that energy increases from symmetric to asymmetric stretching. Whale et al. found that in some intramolecular O–H stretching modes of ice XV, only one O–H bond vibrates, while the other remains static in the molecule. Similarly, we found that only one single O–H bond vibrates in this mode, as shown by the peak at 3424 cm$^{-1}$. We also observed this phenomenon in other ice phases$^{22,24}$ and attributed it to lattice deformation in the local tetrahedral structure. Salzmann et al. reported five Raman peaks at 3190, 3297, 3326, 3360, and 3413 cm$^{-1}$, which are in good agreement with the normal mode peaks at 3196, 3294, 3314, 3342, and 3424 cm$^{-1}$, respectively. The PDOS peaks at 3199, 3300, and 3417 cm$^{-1}$ are also in good agreement with the INS peaks at 3200, 3297, and 3414 cm$^{-1}$, respectively.$^{22}$

IV. CONCLUSIONS

In summary, we used first-principles DFT calculations to simulate the Raman, IR, and PDOS spectra of ice XIII. Based on the good agreement with experimental data, we focused on the relationship between the vibrational peaks and H-bond vibrational modes in the far-IR region from 230 to 330 cm$^{-1}$. Using a self-compiled program, we classified the H-bond modes into strong and weak programs. We also observed this phenomenon in other ice phases as shown by the peak at 3424 cm$^{-1}$. We also found that only one single O–H bond vibrates in this mode, particularly, we found that only one single O–H bond vibrates in this mode, as shown by the peak at 3424 cm$^{-1}$. We also observed the “isolated O–H vibration” phenomenon in other ice phases.

SUPPLEMENTARY MATERIAL

See the supplementary material S1 for the self-compiled program to distinguish the 3D distribution of H-bond vibration and S2 for eight videos (mp4) of the dynamic processes illustrated in Figs. 3 and 4.

ACKNOWLEDGMENTS

The numerical calculations were done on the supercomputing system in the Supercomputing Center, Shandong University, Weihai.

REFERENCES

1. E. Bertie and E. Whalley, J. Chem. Phys. 46, 1271–1284 (1967).
2. E. Bertie, L. D. Calvert, and E. Whalley, J. Chem. Phys. 38, 840–846 (1963).
3. W. F. Kuhs, J. L. Finney, C. Vettiger, and D. V. Bliss, J. Chem. Phys. 81, 3612–3623 (1984).
4. E. Whalley, J. B. R. Heath, and D. W. Davidson, J. Chem. Phys. 48, 2362–2370 (1968).
5. Y. Tajima, T. Matsuo, and H. Suga, Nature 299, 810–812 (1982).
6. K. R. Hirsch and W. B. Holzapfel, J. Chem. Phys. 84, 2771–2775 (1986).
7. C. Lobban, J. L. Finney, and W. F. Kuhs, Nature 391, 268–270 (1998).
8. C. G. Salzmann, P. G. Radaelli, A. Hallbrucker, E. Mayer, and J. L. Finney, Science 311, 1758–1761 (2006).
9. C. G. Salzmann, P. G. Radaelli, A. Hallbrucker, E. Mayer, and J. L. Finney, Phys. Rev. Lett. 103, 105701 (2009).
10. A. Falenty, T. C. Hansen, and W. F. Kuhs, Nature 516, 231–233 (2014).
11. L. del Rosso, M. Celli, and L. Ulivi, Nat. Commun. 7, 13394–13400 (2016).
12. M. Millot, F. Coppa, J. B. Rygg, A. C. Barrios, S. Hamel, D. C. Swift, and J. H. Eggert, Nature 569, 251–259 (2019).
13. C. G. Salzmann, A. Hallbrucker, J. L. Finney, and E. Mayer, Phys. Chem. Chem. Phys. 8, 3088–3093 (2006).
14. C. G. Salzmann, P. G. Radaelli, J. L. Finney, and E. Mayer, Phys. Chem. Chem. Phys. 10, 6313–6324 (2008).
15. M. Martin-Conde, L. G. MacDowell, and C. Vega, J. Chem. Phys. 125, 116101 (2006).
16. S. K. Yao, P. Zhang, Y. B. Lu, H. W. Luo, and Z. J. Zhao, J. Raman Spectrosc. 7, 3612–3623 (2017).
17. K. Zhang, P. Zhang, Z. R. Wang, X. L. Zhu, Y. B. Lu, C. B. Guan, and Y. H. Li, Molecules 23, 1781 (2018).
18. Z. R. Wang, X. L. Zhu, L. Jiang, K. Zhang, H. W. Luo, Y. Gu, and P. Zhang, Materials 12, 246 (2019).
19. X. L. Zhu, Z. Y. Yuan, L. Jiang, K. Zhang, Z. R. Wang, H. W. Luo, Y. Gu, J. W. Cao, X. L. Qin, and P. Zhang, New J. Phys. 21, 043054 (2019).
20. P. Zhang, L. Tian, Z. P. Zhang, G. Shao, and J. C. Li, J. Chem. Phys. 137, 044504 (2012).
21. P. Zhang, S. H. Han, H. Yu, and Y. Liu, RSC Adv. 3, 6646–6649 (2013).
22. L. Jiang, S. K. Yao, K. Zhang, Z. R. Wang, H. W. Luo, X. L. Zhu, Y. Gu, and P. Zhang, Molecules 23, 2780 (2018).
23. S. K. Yao, P. Zhang, Y. Zhang, Y. B. Lu, T. L. Yang, B. G. Sun, Z. Y. Yuan, and H. W. Luo, RSC Adv. 7, 31789–31794 (2017).
24. T. F. Whale, S. J. Clark, L. J. Finney, and C. G. Salzmann, J. Raman Spectrosc. 44, 290–298 (2013).
25. S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. I. J. Probert, K. Refson, and M. C. Payne, Z. Kristallogr. - Cryst. Mater. 220, 567–570 (2005).
26. B. Hammer, L. R. Hansen, and J. K. Korsvold, Phys. Rev. B 59, 7413–7421 (1999).
27. Y. Gu, X. L. Zhu, L. Jiang, J. W. Cao, X. L. Qin, S. K. Yao, and P. Zhang, J. Phys. Chem. C 123, 14880–14883 (2019).
28. J. D. Bernal and R. H. Fowler, J. Chem. Phys. 1, 515 (1933).
29. J. C. Li, J. Chem. Phys. 105, 6733–6735 (1996).
30. B. Mineeva-Sukarova, W. F. Sherman, and G. R. Wilkinson, J. Phys. C: Solid State Phys. 17, 5833–5850 (1984).