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دراسة مركبات شائبة الاكسجين مع الفجوة في الالماس باستخدام نظرية كثافة دالة الدالة

[1*]Khaled M. Etmimi,[2]Asma M. Abotruma, [3]Adel. M. Altameimi , [4]Mohamed. K. Atomi and [5]Fadil. E. Shrif
1 Physics Department, Faculty of Science, University of Tripoli, Tripoli, Libya.
2 High Institute for Comprehensive Professions, Tripoli, Libya.
3 College of Engineering Technology, Tripoli, Libya.
4 Physics Department, Faculty of education, University of Tripoli, Tripoli, Libya.
5 The Libyan Academy, Tripoli, Libya.

*Corresponding: k.emimi@uot.edu.ly

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الملخص:

تبحث هذه الدراسة في خصائص العيوب المرتبطة بوجود فجوة أو أكثر إلى جانب ذرّة الأكسجين في الماس باستخدام نظرية الكثافة الوظيفية، وقد تم نمذجة مركب يتكون من فجوة إلى جانب ذرة أكسجين (O-V) وفجوتي أكسجين ($O\text{-}V_2$) لفهم بنيتها الإلكترونية واستقرارها وارتباطها المحتمل بمراكز الرنين المغناطيسي الإلكتروني (EPR) المعروفة. ويُظهر مركب O-V، الذي يتساوى إلكترونيًا مع مركز فجوة-النيتروجين (NV) الذي تمت دراسته جيدًا في السابق تناظرًا C_{3v} وحالة أساسية ذات دوران مغزلي 1. كما تمت مقارنة متجهات التفاعل الفائق الدقة المحسوبة لذرات ^{17}O وذرات ^{13}C المجاورة بالبيانات التجريبية المستمدة من مركز الرنين المغناطيسي الإلكتروني (EPR) المسمى WAR5، مما يشير إلى احتمال وجود ارتباط بالنسبة لمركب $O\text{-}V_2$، أيضا وجد أن ترتيب V-O-V أكثر استقرارًا من V-V-O بمقدار 0.3 الكترون-فولت، مع حالة أساسية ذات دوران 1 وتناظر C_{2v}. في حين أن الترتيب V-O-V يشترك في بعض أوجه التشابه مع مركز EPR المسمى R5 . وتوفر هذه النتائج رؤى ثاقبة حول البنية الذرية وخصائص العيوب المرتبطة بالأكسجين في الماس، والتي تهم تطبيقات المعلومات الكمومية والاستشعار.

الكلمات المفتاحية:. من البداية، نظرية الدالة الوظيفية، الماس، الأكسجين، الفجوة، التفاعل الفائق الدقة.

A density functional theory study of oxygen-vacancy complexes in diamond

A B S T R A C T:

This study investigates the properties of oxygen-vacancy and –divacancy defects in diamonds using ab initio density-functional theory. Oxygen-vacancy (O-V) and oxygen-divacancy ($O\text{-}V_2$) complexes are modeled to understand their electronic structure, stability, and potential correlation with known electron paramagnetic resonance (EPR) centers. The O-V complex is iso-electronic to the well-studied nitrogen-vacancy $(NV)^{-1}$ center, exhibits C_{3v} symmetry and a spin-1 ground state. Calculated hyperfine tensors for ^{17}O and neighboring ^{13}C atoms are compared with experimental data from the EPR center called WAR5, suggesting a possible association. For the $O\text{-}V_2$ complex, the V-O-V arrangement is found to be more stable than V-V-O by 0.3 eV, with a spin-1 ground state and C_{2v} symmetry. While V-O-V shares some similarities with the EPR center called R5. These findings provide insights into the atomic structure and properties of oxygen-related defects in diamond, which are of interest for quantum information and sensing applications.
Keywords: ab initio, DFT, diamond, oxygen, vacancy, hyperfine interaction

Introduction

Due to their exceptional physical characteristics, diamonds may find applications in electronics that are not feasible when employing silicon or any alternative semiconductor material. However, it is currently possible to create n-type diamonds that contain phosphorus during chemical vapor deposition (CVD) [1] or by ion implantation [2]. The ionization energy of this donor level is 0.62 eV [3]. If one wishes to make electronic devices commercially, shallow donor levels are required.

Given the comparable atomic dimensions of carbon, it is anticipated that oxygen serves as a significant impurity within diamonds. The combustion process may reveal high concentrations of oxygen in the natural diamonds [4]. However, a small percentage (0.04%)

of natural oxygen is ^{17}O [5] which is consistent with little evidence of the involvement of oxygen in EPR centers in diamonds [4,6]. The N3 and OK1 centers have been suggested to contain oxygen, the former in a nearest neighbor nitrogen-oxygen pair, and the latter in a second nearest neighbor nitrogen-oxygen pair [7].

Single vacancies and self-interstitials were produced by irradiating diamond with high-energy particles. Interstitials can be removed by annealing process at a relatively low temperature of approximately 400 ºC [8], whereas the lattice vacancy becomes mobile during annealing at about 600 ºC [9,10]. This leads to the vacancy being trapped by another intrinsic defect, such as a vacancy in irradiated pure diamond, or an extrinsic defect, such as nitrogen or possibly oxygen, if present. The electron-irradiation of type IIa diamond after annealing at different temperatures (up to 1400 ºC) produces several centers that are believed to be formed by the trapping of mobile vacancies at impurities in the <1 1 0> direction of the (110) planes and an effective spin of one [11]. A neutral vacancy in type IIa diamond has an $a^2{}_1t^2{}_2$ electronic configuration, which is introduced from a set of linear combinations of four carbon dangling bond orbitals [12]. This is attributed to the 1.673 eV optical line (labeled GR1) and is EPR-active in the S=1 configuration excited state [13].

It has suggested that the two EPR centers, R5 and R9, may contain complexes of oxygen-divacancy and oxygen-vacancy pairs [8,11], respectively. However, another study [5,11] showed that the R5 center may contain a three-chain vacancy. As mentioned previously, the EPR centers described in implantation studies revealed a thermally stable center labeled KUL12, which is thought to exhibit ^{17}O hyperfine interactions at an axially symmetric center with $A_{||}$=-362 MHz and $A\perp$=-315 MHz.

O-V is an iso-electronic of the well-known N-V^{-1} center, which is EPR and optically active, and has received significant attention in quantum information implementation [14].

The WAR5 EPR center in diamond is a defect primarily observed in samples grown using specific CVD methods that include oxygen. This defect is associated with the O-V, S=0 spin state, although the absence of a ^{17}O hyperfine structure complicates its characterization [15]. In this study, we present the results of density functional simulations regarding the structure, electrical levels, and electronic structures of the oxygen-vacancy and oxygen-di-vacancy complexes in diamond. We also investigate hyperfine tensors in comparison to the suggested EPR centers in the literature where possible.

Method

We employed the ab initio density-functional theory method as implanted in the AIMPRO code [16,17]. In all calculations, we employed the exchange-correlation potential using the generalized gradient approximation [18]. The Brillouin-zone was sampled using the Monkhorst-Pack scheme [19] with a uniform mesh of 2×2×2 special k-points. For representative cases, we have compared total energies with a 4×4×4 mesh, and the results suggest our values from the smaller mesh are converged to the order of 10 meV with respect to the Brillouin-zone sampling.

The Kohn-Sham wavefunction was expanded using a Gaussian-type orbital basis [20]. Carbon and oxygen were treated using fixed linear-combinations of s- and p-orbitals with the addition of a set of d-functions to allow for polarization, with a total of 22 functions per atom. The charge density used plane-waves with a cut-off of 300 Ha, yielding well converged total energies. Generally, 216-atom, simple-cubic supercells of side length $3a_0$ are used. Climbing nudged elastic bands [21,22] were used to obtain diffusion barriers. Core-electrons are eliminated by using pseudo potentials [23], so that hyperfine interactions are

obtained by reconstructing the all-electron wave functions in the core region [24,25]. The atomic calculations for the reconstruction of the hyperfine calculations were performed using a systematic polynomial basis [26]. The electrical levels were calculated using the marker method by comparing the acceptor and donor with boron and nitrogen, respectively.

The results

Oxygen vacancy complex

Impurity-vacancy complexes often exhibit active optical and electrical properties. The well-known complex N-V is giving rise to a zero-phonon line at 1.945 eV (637 nm) [27] and optical centers at 2.156 eV (575 nm) [28] in the neutral and negative-charged states, respectively. O-V is an iso-electronic of $N\text{-}V^{-1}$. Unlike O-V in silicon [29], there is very little information on O-V pair in diamond.

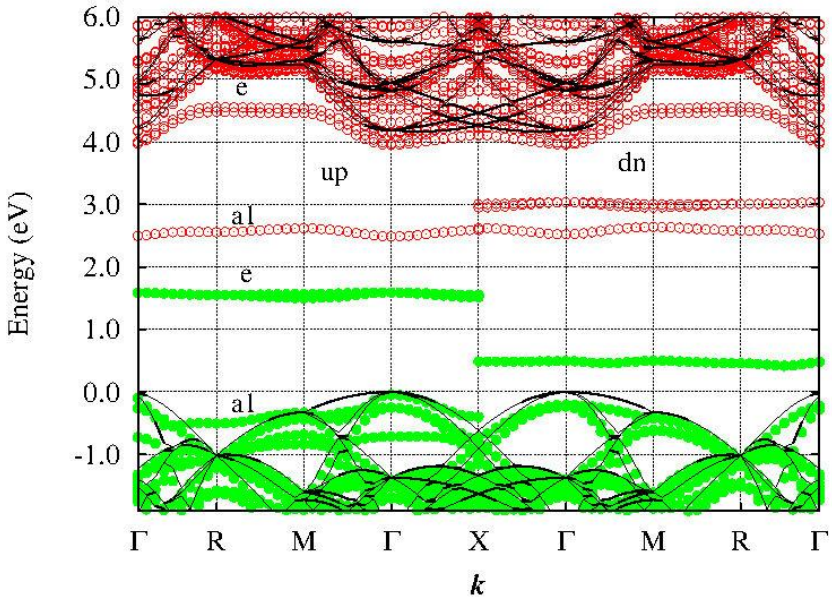

Figure 1: Band structure for the S=1 configuration of the O-V complex in diamond. Filled and empty circles show filled and empty bands respectively. The energy scale is defined by the valence band top at zero energy E_v=0 eV. With spin-up bands on the left-hand panel and spin-down bands on the right. The underlying solid bands are taken from a defect-free supercell of the same size.

O-V with an S=1 spin configuration gives rise to $a_1^2e^2a_1^0e^0$ electronic levels in the vicinity of the band gap. In addition to the filled levels$a_1^2e^2$ which are similar to the band gap of NV^{-1}, there is a degenerate empty level and one singlet empty level.

The singlet a_1^0 level represents an antibonding orbital that belongs to the oxygen-carbon bonding interactions as shown in Fig. 1, which is consistent with previous theoretical work [30,31]. It was expected that O-V would exhibit more optical transitions compared to $N\text{-}V^{-1}$.

Electrical levels calculated using the marker method [32,33]. We use nitrogen and boron as donor and acceptor references, respectively, give the donor level of O-V at E_c-3.3 eV and the acceptor level at E_v+3.1 eV. Since the donor level of substitutional nitrogen (N_s) lies above the acceptor level of O-V, so charge transfer is expected to occur in type Ib natural

diamond which, give rise to negatively charged defects. In the negative charged state, the spin S=3/2 is more stable than spin S=1/2 by just 0.03 eV in contrast with Ref. [34]. While in the positive charged state, it is found that the spin S=1/2 is more stable than the spin S=3/2 by 0.9 eV.

Our calculation shows that the binding energy of the oxygen-vacancy pair possess a configuration more stable than isolated oxygen and vacancies by 4.6 eV where the formation energy of V has been taken to be 6 eV from quantum Monte Carlo calculations [35] because it is difficult to calculate accurately by the present method due to multiplet energies, whereas O-V preferred to be S=1 spin state configuration over S=0 by 0.36 eV energy different and both have C_{3v} symmetry group. Because O_s has the acceptor level (-/0) lies above the donor level (0/+) of V (the donor level of V located at E_v+0.3 eV according to various studies [32,36,37]). Thus, the reaction of O^-+V^+ is less likely. The other reaction might be O^++V^-, where the (0/+) of O_s lies above the (-/0) of V.

Table 1. Calculated hyperfine tensors (MHz) of ^{17}O and three identical ^{13}C with three fold-coordinators in O-V complexes, $S = 1$. θ and ϕ are given relative to the directions [001] and [100] respectively.

Site	A_1		A_2		A_3	
Experimental: WAR5, C_{3v}, $S = 1$ [15,34]						
3a	197.4	(54,225)	117.3	(36,45)	118.2	(90,135)
6g	17.5	(60,225)	11.7	(30,45)	13	(90,135)
3l	12.6	(55,225)	8.5	(35,45)	8.5	(90,135)
3c/3h	7.4	(55,225)	4.3	(35,45)	4.3	(90,135)
Calculations: O-V, C_{3v}, $S = 1$						
3a	208	(54, 225)	121.93	(36, 45)	122	(90, 135)
6g	19.17	(54, 222)	13.08	(139, 188)	13.23	(72, 119)
3l	18.07	(57, 225)	12.43	(33, 45)	12.26	(90, 135)
3c	−7.55	(84, 45)	−9.56	(6, 225)	−9.76	(90, 135)
^{17}O	14.4	(55, 225)	16.4	(35, 45)	16.4	(90, 135)
Calculations: $(N\text{-}V)^{-1}$, C_{3v}, $S = 1$						
3a	209.42	(125, 46)	123.75	(135, 180)	123.49	(65, 118)
^{14}N	−1.77	(55, 315)	−2.25	(90, 45)	−2.25	(35, 135)
Experimental: $(N\text{-}V)^{-1}$, C_{3v}, $S = 1$ [38]						
	$A_\parallel$		$A_\perp$			
3a	199.7	(125.26, 45)	120.3	–		
^{14}N	−2.14	–	−2.70	–		
Calculations: $(O\text{-}V)^{+1}$, C_s, $S = 1/2$						
2a	360.31	(126, 225)	188.02	(52, 282)	188.54	(58, 162)
1a	−190.47	(55, 315)	−97.60	(114, 26)	−96.75	(135, 270)
^{17}O	−2.41	(70, 201)	0.33	(135, 270)	1.93	(52, 308)
Calculations: $(O\text{-}V)^{-1}$, C_s, $S = 3/2$						
2a	139.63	(55, 314)	82.33	(99, 38)	82.44	(36, 115)
1a	137.08	(126, 45)	81.58	(90, 315))	81.63	(144, 225)
^{17}O	−181.12	(155, 45)	−161.28	(65, 45)	−154.69	(90, 315)

EPR data showed that an R9 [8,11,39] center of orthorhombic symmetry might be an O-V pair. However, there is no direct evidence for the presence of oxygen in this center. Moreover, our calculations showed that this center gained C_{3v} symmetry. The R9 center was observed with three main spectra (R4, R5, and O1) by studying electron-irradiated type IIa diamond followed by annealing at various temperatures up to 1400 ºC [11]. It was not possible to determine whether the spin state of R9 is S=3/2 or S=1 due to a line from other centers being present in the middle of the spectrum. The symmetry of R9 is identified as orthorhombic-I [8], which disagrees with the C_{3v} identified in the present work. Another

EPR center called R12 with trigonal symmetry has been suggested to arise from O-V. O-V has C_{3v} symmetry and S=1, which is consistent with the R12 EPR center but not with R9.

Although the low abundance of ^{17}O reduces the chances of experimentally detecting O as an EPR center, hyperfine calculations for ^{17}O and threefold coordinated carbon atoms are shown in Table [1]. As mentioned above, the O-V complex resembles the $(N\text{-}V)^{-1}$ in terms of electronic structure, and the hyperfine calculations.

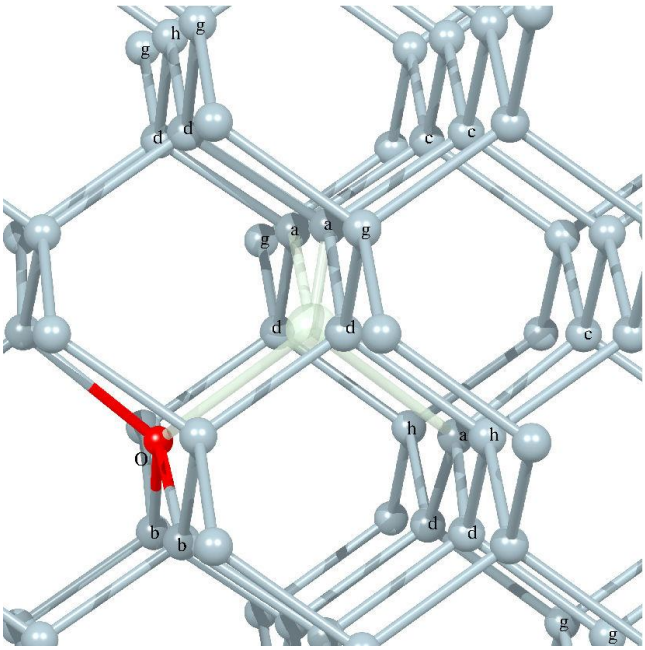

Figure 2: Schematic structures of the oxygen-vacancy complex at S=1 spin state. gray and red spheres represent C and O, with transparent sphere showing the vacant site.

The comparison of the hyperfine of the threefold coordinated carbons in $(N\text{-}V)^{-1}$ with that of O-V shows relatively similar values of hyperfine on carbon atoms neighboring the oxygen, which means that the amount of spin density on radical carbon sites is the same as that of the $(N\text{-}V)^{-1}$. In the positively charged state, the hyperfine values of O are relatively small, indicating that the spin density is localized in the vicinity of three carbon radical atoms, where the structure symmetry is reduced from C_{3v} to C_s making one O-C bonds longer than the other two. The hyperfine values on long O-C antibonds are halved compared to those on two short bonds. However, in the negatively charged state, the spin density is localized on the anti-bond between three carbon atoms neighboring the oxygen, increasing the spin density on O, which leads to larger O-related hyperfine values in contrast to previous ab inito study [34].

Another EPR center, called WAR5, was observed by Cann [15], where the general features of the WAR5 center are oxygen atoms trapping a vacancy in the neutral charge state. WAR5 has been examined previously, and we review only the main points here. The defect has been shown to possess S=1 electronic spin and C_{3v} symmetry. This center was found in a CVD diamond, which was grown from an experimental chemistry containing oxygen. However, the presence of oxygen has not yet been confirmed due to the low natural abundance of ^{17}O. Cann [15] suggested that a few atoms were responsible for the WAR5

center, and the oxygen atom was strongly suggested. It is necessary for the impurity atom neighboring vacancy to have a low natural abundance of $I \neq 0$ isotopes; otherwise, hyperfine interactions would have been detected. Moreover, for large atoms, it is energetically favorable to adopt split-vacancy formation, which does not display C_{3v} symmetry. In our study on the WAR5 center, oxygen impurity atom has been considered as candidates. Four sets of ^{13}C hyperfine satellites from the main transition are listed in Table 1. These satellites are denoted as `a', `g', `l', and `c' as a reference to a study on $(NV)^{-1}$ conducted by Felton [38] and Cann [15].

Small spin density can be found on the oxygen atoms whereas the majority of the spin density is localized on the three carbons sp^3 dangling bonds neighboring the vacancy, which is denoted as `a'. The hyperfine interactions for the `a' and six equivalent C atoms `g' were tilted slightly off the crystallographic direction by about 1°. The detailed values and directions of these hyperfine interactions are provided in Table [1]. The experimental hyperfine tensors of neutral charged O-V S=1 match well with the theoretical calculations, supporting the characterization of the defect. Moreover, compared with simulations using density functional theory by Thiering [34], we found that the calculated hyperfine tensors of neutral O-V S=1 agree well, as listed in Table [1].

Oxygen-divacancy complex

As mentioned above, little information is available regarding the O-V complex. The EPR center, called R5, was suggested to be an O-V_2 structure. However, the arrangement has not been suggested yet. Interestingly, the V-O-V (Fig. 3 (a)) arrangement is more favorable than V-V-O (Fig. 3 (b)) by 0.3 eV, and the triplet spin state configuration is more stable than singlet by 0.5 eV. The V-O-V structure has one extra carbon atom with three-fold coordination i.e., an extra dangling bond, whereas V-V-O has three-fold coordinated with oxygen rather than two-fold coordinated in the V-O-V structure. Energy saving can be explained from electronic structures. The band gap (plotted in Fig. 4 (a) and (b)) shows that V-O-V has the highest filled level which is lower than that of V-V-O. Moreover, the separation between the highest two filled levels is more than that for V-V-O which almost degenerates in the band gap. The activation energy for the reorientation of the oxygen atom from V-O-V to V-V-O is 2.7 eV, indicating that it is unlikely to obtain a structure from one to another. The binding energies have been considered for the formation of V-O-V. First, O-V+V, could be formed by O-V trapping a second vacancy.

(a) (b)

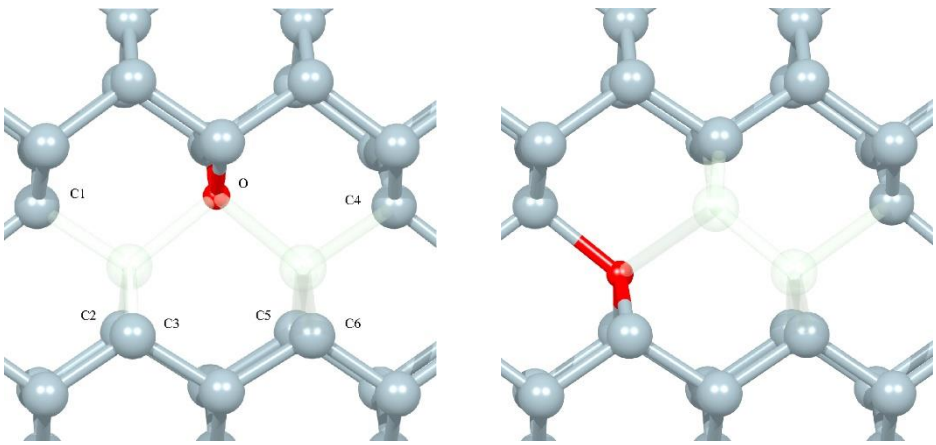

Figure 3: Schematic structures of (a) the vacancy-oxygen-vacancy complex and (b) the oxygen-vacancy-vacancy. Grey and red spheres represent C and O, with transparent spheres showing vacant sites.

The binding energy to form such a structure is 3.7 eV relative to the separated O-V and single V. The second is divacancy+oxygen, which is more favorable than separated divacancy and oxygen by about 8.3 eV. Therefore, in dissociation, O-V_2 could end up with O-V+V. The acceptor level at E_v+2 eV is below the donor level of N_s and so, in agreement with the case of O-V, a negatively charged state can occur. The donor level is at E_c-3.8 eV in the band gap, which is deep in the gap, thus shallow acceptor cold ionized the defect. In the positively charged state, it is found that S=1/2 spin state is more stable than S=3/2 spin state by 0.9 eV, whereas in the negatively charged state, S=3/2 is more stable than S=1/2 by just 0.5 eV.

V-O-V has C_{2v} symmetry and S=1 spin state consistent with the R5 EPR center which has been indeed suggested to be the O_sV_2 center [8]. However, other studies [5,11] conducted with either type IIb diamond or free nitrogen single crystals irradiated by ^{17}O ions have suggested that R5 is a chain of three vacancies in the [110] direction. V-O-V are EPR active since has the S=1 configuration. Table 2 illustrates the hyperfine tensors on ^{17}O and six three-fold coordinated carbon atoms in different charged states. Neither arrangement agrees with the experimental results of ^{13}C hyperfine values [5,40] in terms of hyperfine tensors. In three different charged states, the unpaired electron probability density is localized on four equivalent carbon atoms that are not in the (110) plane containing the two vacancies and oxygen and with smaller (about half of the values) on the remaining two carbon atoms in the plane.

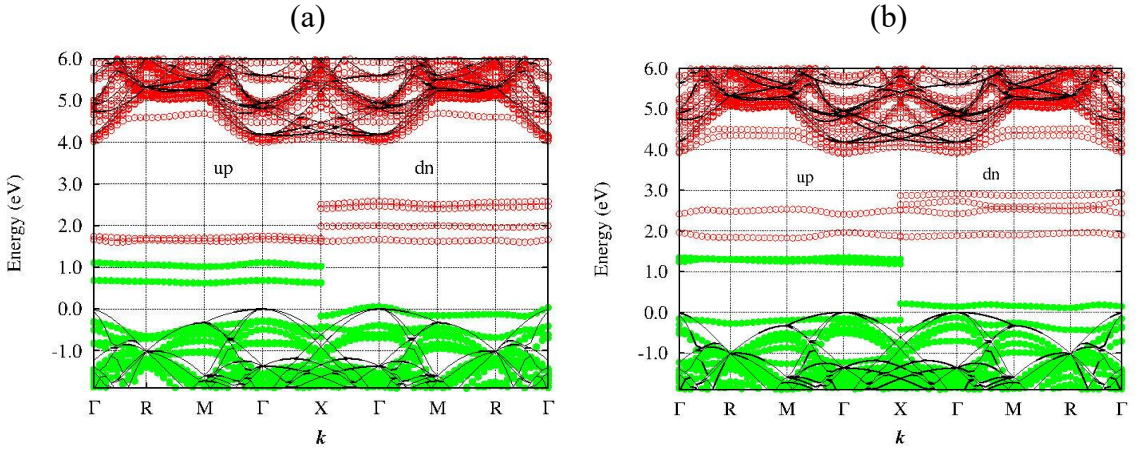

Figure 4: Band structure for the S=1 configuration of (a) the V-O-V complex (b) V-V-O complex. Filled and empty circles show filled and empty bands respectively. The energy scale is defined by the valence band top at zero energy E_v=0 eV. With spin-up bands on the left-hand panel and spin-down bands on the right. The underlying solid bands are taken from a defect-free supercell of the same size.

Table 2. Calculated hyperfine tensors (MHz) of ^{17}O and six ^{13}C with three fold-coordinators in V-O-V complexes. θ and ϕ are given relative to the directions $\langle 001 \rangle$ and $\langle 100 \rangle$ respectively.

Site	A_1		A_2		A_3	
Calculations:V-O-V, $S = 1$, C_{2v}						
^{17}O	-10.75	$(90, 180)$	-8.22	$(45, 90)$	3.04	$(135, 90)$
C1 and C4	-103.29	$(54, 226)$	-54.85	$(114, 154)$	-54.48	$(45, 90)$
C2,C3,C5, and C6	191.77	$(55, 224)$	103.18	$(145, 215)$	101.97	$(94, 311)$
Calculations:$(\text{V-O-V})^{+1}$, $S = 1/2$, C_{2v}						
^{17}O	-11.62	$(90, 270)$	-7.69	$(45, 180)$	6.99	$(135, 180)$
C1 and C4	-107.05	$(126, 136)$	-52.19	$(67, 64)$	-51.82	$(135, 0)$
C2,C3, C5 and C6	231.51	$(52, 137)$	127.59	$(88, 45)$	128.41	$(142, 132)$
Calculations:$(\text{V-O-V})^{-1}$, $S = 3/2$,C_{2v}						
^{17}O	1.03	$(90, 270)$	1.24	$(45, 0)$	1.90	$(45, 180)$
C1 and C4	63.64	$(56, 313)$	40.37	$(65, 62)$	40.66	$(45, 180)$
C2, C3,C5 and C6	128.26	$(55, 136)$	73.47	$(96, 51)$	74.41	$(144, 149)$

Conclusions

In general, O-V gives rise to a low-lying a_1 energy level and a higher lying doubly degenerate *e* level occupied by four electrons. In addition, there are two other levels, the unoccupied a_1 level near the middle of the energy gap and empty *e* level emerges close to the conduction band minimum (CBM). The former constitutes an antibonding orbital localized at the oxygen-carbon bonds. O-V defect exhibiting C_{3v} symmetry with a S = 1 triplet ground state closely resembles that of the nitrogen vacancy $(NV)^{-1}$ as two electrons will inhabit the doubly degenerate *e* level. Although no strong evidence in relation to the O-V and V-O-V models in terms of EPR centers is presented here, there are consistencies in terms of spin state and symmetry points with R12 and R5 [8], respectively. WAR5 EPR center with a specific spin state and symmetry was tentatively associated with O-V S=1 defects. However, the impurity atom neighboring a vacancy must exhibit a minimal natural abundance of nuclear spin $I \neq 0$ isotopes; otherwise, due to the signal intensity, hyperfine interactions will not be observable. This observation is consistent with the existence of the oxygen atom, where no hyperfine interaction would be observed due to the 0.038% natural abundance of I =5/2 of ^{17}O. Moreover, for larger atoms, it is energetically advantageous to adopt a split-vacancy formation [30], which does not exhibit C_{3v} symmetry, such as a silicon split vacancy [41]. Consequently, to maintain its position at the substitutional site, the impurity atom must not be too large. This is consistent with the oxygen atom, which has atomic dimensions similar to those of carbon atoms, supporting the O-V with S=1 characterization.

In terms of the stability of the oxygen-divacancy complex, the most surprising case is that the arrangement V-O-V is found to be more stable than V-V-O, which has one less dangling bond. While oxygen formed one more bond with neighboring carbon atoms in the latter.

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