Excited states in hydrogenated single-layer MoS$_2$

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Abstract
Our calculations of the excitation spectrum of single-layer MoS$_2$ at several hydrogen coverages, using a density-matrix based time-dependent density-functional theory (TDDFT) show that the fully hydrogenated system is metallic, while at lower coverages the spectrum consists of spin-polarized partially filled localized mid-gap states. The calculated absorption spectrum of the system reveals standard excitonic peaks corresponding to the bound valence-band hole and conduction-band electron, as well as excitonic peaks that involve the mid-gap states. Binding energies of the excitons of the hydrogenated system are found to be relatively large (few tens of meV), making their experimental detection facile and suggesting hydrogenation as a knob for tuning the optical properties of single-layer MoS$_2$. Importantly, we find hydrogenation to suppress visible light photoluminescence, in agreement with experimental observations. In contrast, both Li and Na atoms transform the system into an n-doped non-magnetic semiconductor that does not allow excitonic states.

Keywords: excitation spectrum, optical properties, excitons, absorption and emission spectrum

(Some figures may appear in colour only in the online journal)

1. Introduction
Offering versatile electronic and optical properties, two-dimensional (2D) transition metal dichalcogenides (TMDCs) have attracted much interest. They exhibit attractive properties such as strong photoresponse and transition from indirect to direct band gap as the number of atomic layers decreases to one [1–3]. Furthermore, the bandgap of 2D TMDCs may be tuned quantitatively by varying the layer thickness and strain [4,5]. They may also show edge-structure dependent semiconducting-to-metallic transitions [6]. At the same time, adsorption of an alkali metal (K) atoms has been shown to have significant influence on the catalytic properties of MoS$_2$ [7–10], while the exposure of Na to the MoS$_2$(0001) surface leads to expected n-type dopant shifts of the bands [11–13], which is to be contrasted with the effect of Co atoms on the electronic structure of WSe$_2$(0001) [13]. While Na atoms act as electron donors in MoS$_2$, Co atoms serve as electron acceptors (p-type) in WSe$_2$. These dopants dramatically modify the electronic structure of these materials, and thus their excitation spectrum (for example, by enhancing plasmonic properties through increased density of carriers). Hydrogenation was found to affect the structural, electronic, optical, magnetic and catalytic properties of 2D TMDCs [14]. It could also change the intrinsic n-doping to p-doping, at room temperature, and completely saturate sulfur vacancies in MoS$_2$ flakes [15]. Hydrogenation may also lead to a quench of the photoluminescence (PL) of single-layer MoS$_2$ [16]. The above properties are, of course, temperature dependent. For example, a 500 °C heat treatment restores the electronic and optical properties of the system by stimulating desorption of the hydrogen atoms [17]. Other 2D TMDCs, such as monolayer MoSe$_2$, have also responded to hydrogenation via a plasma treatment [17] inducing a charge transfer from hydrogen to MoSe$_2$ which changes the electronic and excitation properties of the system, resulting in a shift of the PL peak and a ∼3-fold decrease of the electron mobility.

Significant advances in understanding some of the above properties of hydrogenated monolayer MoS$_2$ have been made through application of density functional theory (DFT). It
was shown that electronic structure and magnetism of hydrogenated monolayer MoS$_2$ can be modified under uniaxial tensile strain [18]. Furthermore, magnetic properties of monolayer MoS$_2$ were found to depend strongly on hydrogen concentration and adsorption sites: adsorption at the center of the hexagonal ring with a relatively high concentration of H atoms produces itinerant ferromagnetism, while adsorption on sulfur atoms with a low concentration of H atoms yields flat-band ferromagnetism [19]. Interestingly, in the latter case, it was found that the electrons are distributed on H and neighbor Mo and S atoms, while in the non-magnetic case they are mostly localized on the Mo atoms neighboring hydrogen. Another consequential finding is that hydrogenation significantly reduces diffusion barriers for Ni and S complexes and helps build stable conducting nanorods on MoS$_2$ [20]. DFT calculations have also shown [21] that the interaction of H with MoS$_2$ becomes more favorable with increasing hydrogen concentration. Absorption of a single H per $4 \times 4 \times 1$ cell produces a mid-gap state approaching the Fermi level, and hence significantly increases the n-type carrier concentration and as result the system’s electrical conductivity.

The interplay of spin-valley coupling, orbital physics, and magnetic anisotropy in several 2D TMDCs with a single adsorbed magnetic transition-metal (TM) atom was exploited by Shao et al [22] to demonstrate that the spin-flip scattering rates in the systems depend strongly on the involved orbitals, since orbital selection rules define the kinetic exchange coupling between the adatom and the charge carriers. These findings point to potential spintronic application by tuning magnetic and spin transport properties via doping with TM adatoms. Quite remarkably, it was shown theoretically that another hydrogenated 2D material—single layer h-BN—demonstrates an oscillatory dependence of the bandgap on hydrogen concentration, making it possible to tune absorbptive and emissive properties of the system [23]. DFT studies of adsorptive properties of monolayer TMDCs [24] have also shown that surface and interlaminar hydrogenations have different effects on electronic properties: in several systems surface hydrogenation induces magnetism and reduces the bandgap, but does not modify the semiconducting character of the monolayer, while interlaminar hydrogenation induces a semiconductor-to-metal transition. Moreover, it has been shown theoretically that, akin to graphene, hydrogenation might significantly enhance the critical temperature and superconducting properties of 2D materials [25,26]. These results demonstrate a potential of hydrogen functionalization of TMDCs for use in electronic and magnetic devices.

In the experimental and theoretical results described above the excitation spectrum of hydrogenated MoS$_2$ plays a very important role. It is thus somewhat surprising that there is a lack of an ab initio study of the effect hydrogenation on the excitation spectrum of MoS$_2$. To provide this much needed microscopic understanding, we have performed a combined DFT and TDDFT study of the excitation spectrum of hydrogenated single-layer MoS$_2$ by paying special attention to changes in the excitonic properties as a function of coverage of hydrogen atoms. In addition, we analyze the electronic properties of single-layer MoS$_2$ under adsorption of two other atoms with a single s electron in the outer shell—Li and Na. As we shall see, only H as an adsorbate creates non-hybridized and well-isolated hydrogenic states within the bandgap, bringing forth new excitonic states that enrich the excitonic properties of pristine single-layer MoS$_2$.
Figure 3. Band structure of MoS\textsubscript{2} fully covered with (a) hydrogen (b) lithium (c) sodium, calculated using GGA-PBE. The blue shades represent the contribution of the H, Li, Na-s states and red those of Mo and S orbitals. Here and in figures 5 and 6, the horizontal black lines mark the Fermi energy.

Figure 4. Projected density of states (PDOS) of MoS\textsubscript{2} fully-covered with (a) hydrogen, (b) lithium and (c) sodium atoms. The results are obtained with GGA–PBE.

2. Computational details

We performed calculations based on DFT with the plane-wave and pseudopotential methods as implemented in the Quantum Espresso package [27]. We treated exchange correlation effects within the generalized gradient approximation in the form developed by Perdew–Burke–Ernzerhof (GGA–PBE) [28] and the local density approximation (LDA), as parameterized by Perdew and Zunger (LDA–PZ) [29]. We used ultrasoft pseudopotentials to describe the core-valence electron interactions. We applied kinetic energy cutoffs of 60 Ry and 360 Ry, respectively, for calculations of valence electron wave functions and electron density. We used a 16 × 16 × 1, 6 × 6 × 1, 4 × 4 × 1 Monkhorst–Pack (MP) grid for \textit{k}-point sampling of the Brillouin zone to generate a fine reciprocal-space grid for the 1 × 1 × 1, 3 × 3 × 1 and 5 × 5 × 1 cells, respectively. We optimized atomic positions and lattice parameters, until the residual forces converged to less than 0.01 eV Å\textsuperscript{−1}.

To calculate the excitonic binding energies we used the density-matrix TDDFT approach [30,31], in which the Kohn–Sham equation \( i \frac{\partial \Psi_\mathbf{k}(\mathbf{r}, t)}{\partial t} = \mathbf{H}(\mathbf{r}, t) \Psi_\mathbf{k}(\mathbf{r}, t) \) is solved by using the following ansatz for the wavefunction: \( \Psi_\mathbf{k}(\mathbf{r}, t) = \sum c_\mathbf{k}^l(t) \varphi_0^l(\mathbf{r}) \), where \( \varphi_0^l(\mathbf{r}) \) are the static DFT wavefunctions (\( l \) is the band index, \( k \) is the wave-vector) and \( c_\mathbf{k}^l(t) \) are their time-dependent coefficients. The sum in the ansatz is over all bands involved into the optical transitions. In this work, we use the two-band approximation which reduces the problem to finding bilinear combination of the c-coefficients that constitute the density matrix: \( \rho_{\mathbf{k}l}^{lm}(t) = c_\mathbf{k}^l(t) c_\mathbf{k}^m(t) \). Indeed, the elements of the density matrix define practically all properties of the system—the level occupancies (diagonal elements), electronic transitions (polarization), excitons (non-diagonal elements), etc. The density matrix elements satisfy the Liouville equation: \( i \frac{\partial \rho_{\mathbf{k}l}^{lm}(t)}{\partial t} = \mathbf{H}(\mathbf{r}, t) \rho_{\mathbf{k}l}^{lm}(t) \), where \( \mathbf{H}_{\mathbf{k}l}^{lm}(t) = \int \varphi_0^{l*}(\mathbf{r}) \mathbf{H}(\mathbf{r}, t) \varphi_0^m(\mathbf{r}) \mathrm{d}r \) are the matrix elements of the Hamiltonian with respect to the static wave functions (Kohn–Sham orbitals). From the valence (\( v \)) and conduction (\( c \)) bands one can derive the TDDFT Casida equation [32], in the Tamm–Dancoff approximation [33], for
Figure 5. Band structure of hydrogenated MoS$_2$ at (a) 1/9 coverage and (b) 1/25 coverage obtained with GGA–PBE. Spin-up and spin-down states are shown in red and blue colors, correspondingly.

Figure 6. Band structure of MoS$_2$ for 1/9 coverage of Li (a) and Na (b) atoms.

$\rho_{cv}(\vec{k})$, that describes exciton states by using the linear form of the Liouville equation [30]:

$$\sum_{\vec{k}'} \left[ (\epsilon_{cv}^{\vec{k}} - \epsilon_{cv}^{\vec{k}'} ) \delta_{\vec{k},\vec{k}'} + F_{\vec{k},\vec{k}'} \right] \rho_{cv}^{\vec{k}'}(\omega) = E_{\alpha} \rho_{cv}^{\vec{k}},$$  \hspace{1cm} (1)

where $\epsilon_{cv}^{\vec{k}}$ and $\epsilon_{cv}^{\vec{k}'}$ are the free electron and hole energies at the specific wave vector (providing their energy dispersion), $\rho_{cv}^{\vec{k}'}(\omega)$ is the $N_k$-component of the polarization vector ($N_k$ is the number of points in momentum space), $n$ numbers the excited state, and $F_{\vec{k},\vec{k}'}$ is the TDDFT effective electron-hole interaction:

$$F_{\vec{k},\vec{k}'} = \int d\vec{r}_1 d\vec{r}_2 \phi_{\vec{k}'}^0 (\vec{r}_1) \phi_{\vec{k}}^0 (\vec{r}_2) f_{xc}(\vec{r}_2, \vec{r}_1) \phi_{\vec{k}'}^0 (\vec{r}_2) \phi_{\vec{k}}^0 (\vec{r}_1)$$  \hspace{1cm} (2)

defined by the exchange-correlation (XC) kernel $f_{xc}(\vec{r}_2, \vec{r}_1)$. To obtain the excitonic binding energies, we solve equation (1) using both the long-range (LR) and Slater XC kernels [31], as implemented in the BEE code that we have developed [30,34]. We use periodic boundary conditions along $x$ and $y$-axis and added a 15 Å vacuum along $z$-axis to eliminate the interaction between the model 2D system and its periodic images. To simulate the system with different concentrations of H, Li and Na coverage we used $1 \times 1 \times 1$, $3 \times 3 \times 1$, and $5 \times 5 \times 1$ size supercells, which gave us three adsorbate coverages—full, 1/9, and 1/25, respectively.

The LDA-PZ eigenenergies and $\epsilon_{cv}^{\vec{k}}$ and eigenfunctions $\phi_{\vec{k}}^{\alpha}(\vec{r})$ are used to construct and solve the exciton eigenenergy equation (equation (1)). The solution of equation (1) was obtained for the $k$-point set for the irreducible Brillouin zone. An approach similar to the above when applied to
calculate the exciton and trion binding energies in several TMDCs produced results in reasonable agreement with experimental observations [32].

Once the electronic spectrum and the exciton eigenenergies $E_n$ and the corresponding $(N_i$-component) eigenvectors $\rho_{n,k}^{ci}$ were found by solving equation (1), we calculated the absorption spectrum in the usual manner:

$$A(\omega) = -\mathrm{Im} \frac{1}{\pi} \sum_n \frac{f_n}{\omega - E_n + i \delta}.$$  

(3)

In equation (3) the summation is performed over excited states $n$ between the initial state valence band and final conduction band; $f_n$ is the oscillator strength of the transition [32,35]:

$$f_n = \frac{2}{3} E_n |\bar{d}_n|^2,$$  

(4)

where

$$\bar{d}_n = \langle 0 | \tilde{r} | n \rangle$$

and

$$\sum_k \frac{2 E_0}{E_n} \rho_{n,k}^{cv} \bar{d}_{ck} + \sum_k \frac{2 E_0}{E_n} \rho_{n,k}^{cv} \bar{d}_{ck} = \sum_k \frac{2 E_0}{E_n} \rho_{n,k}^{cv} \bar{d}_{ck} = \sum_k \frac{2 E_0}{E_n} \rho_{n,k}^{cv} \bar{d}_{ck}$$

is the transition dipole moment from the ground (0) to the excited state $n$ and $E_0$ and $E_n$ are, respectively, the energies of the excited state calculated within DFT and TDDFT, respectively. The summation in equation (5) is performed over $N_k$ points on the irreducible zone obtained using the grid scheme as described above, and corresponds to all possible vertical transitions from the valence to the conduction band. Finally, in equation (3) we used $\delta = 0.1$. We calculated both TDDFT and DFT absorption spectra (in DFT one puts in equation (5) $E_n \rightarrow E_0$) and for $\rho_{n,k}^{cv}$—the eigenvectors obtained by solving equation (1) at $E_{F}^{cv} = 0$.

The emission spectra were obtained from the absorption spectrum $A(\omega)$ by multiplying it by the Planck factor [36]:

$$E(\omega) = \frac{4 \pi \omega^4}{e^{\omega/\Delta} - 1} A(\omega),$$  

(6)

where $\Delta$ is the optical gap in the system (the difference between the energy of lowest-excited state and the energy at the top of valence band) and for temperature we used a representative temperature $T = 0.01 \text{ eV}$ (i.e., of order of room temperature). The spectrum at lower temperatures will be similar, but with more narrow peaks.

To sketch the spatial charge distributions of the electron and hole comprising the exciton, we used the fact that the excited charge density can be expressed in terms of the DFT wave functions and Liouville matrix elements as:

$$\delta n(r, t) = \sum_{k<k_F} \left( |\psi_k(r, t)|^2 - |\psi_k(r, 0)|^2 \right)$$

$$= \sum_{k<k_F} \left( \rho_k^{ce}(t) \psi_k^{(0)}(r) \psi_k^{0*}(r) + \rho_k^{ce}(t) \psi_k^{0*}(r) \psi_k^{(0)}(r) \right) + \rho_k^{se}(t) \psi_k^{(0)}(r) \psi_k^{0*}(r).$$

(7)

The first and second terms above correspond to excitation and deexcitation processes, respectively, and the third to the charge in the conduction band. The change of the charge density due to creation of the exciton in state $n$ is:

$$|\psi_{X,n}(r)|^2 = \sum_{k<k_F} \rho_k^{ce}(r) \psi_k^{0*}(r) \psi_k^{0*}(r).$$

(8)

For clarity in visualization of the calculated exciton charge distribution (for $n = 1$), we plotted individual contributions of the electron and hole charges as $\sum_{k<k_F} \rho_k^{ce}(r) \psi_k^{0*}(r)$ and $\sum_{k<k_F} \rho_k^{se}(r) \psi_k^{0*}(r)$ (i.e., by fixing the electron or the hole coordinate to be zero), correspondingly.

### 3. Results and discussion

In this section, we summarize the results of our calculations and their analysis. We first focus on the electronic structure of the pristine and hydrogenated single-layer MoS2. This is followed by considerations of the binding energy of the excitons in section 3.2. In section 3.3 we discuss the calculated absorption and emission spectra of the systems of interest which provides a connection with the observed PL data and finally in
Table 1. Calculated exciton binding energies in meV and corresponding dipole strengths, for two hydrogen coverages for excitons (A-D) defined in figure 8. The dipole strengths are in units of the ‘standard’ excitonic state formed by the valence hole and conduction electron (B in figure 8).

| Exciton | 1/25 Coverage | 1/9 Coverage |
|---------|---------------|--------------|
|         | Slater LR    | Strength     | Slater LR    | Strength     |
| A       | −63.708       | −61.346      | 0.05         | −2.406       | −1.885       | 5            |
| B       | −57.016       | −57.009      | 1            | −1.126       | −0.679       | 1            |
| C       | −82.592       | −97.578      | 47           | −26.771      | −40.25       | 27           |
| D       | −57.043       | −57.053      | 0.1          | −1.054       | −0.834       | 6            |

Figure 9. Comparison of TDDFT (black curves) and DFT (blue curves) results. Top row: absorption (a) and emission (b) spectra of single-layer MoS$_2$. Bottom row: absorption (c) and emission (d) spectra of the MoS$_2$-H system with 1/25 hydrogen coverage.

section 3.4, we examine the details of the charge distribution related to the excitons being investigated. Our conclusions are summarized in section 3.5.

3.1. Electronic structure of pristine and hydrogenated single-layer MoS$_2$

For pristine and hydrogenated single layer MoS$_2$, shown schematically in figure 1, after ionic relaxation, we found the optimized lattice constant to be 3.124 and 3.186 Å, with LDA and PBE, respectively, in a good agreement with previous calculations [37]. The direct bandgap at the K point is $\sim 1.78$ eV and 1.66 eV for LDA–PZ and GGA–PBE, respectively which is also in agreement with previously reported theoretical [38,39] and experimental values [4,40] (though, in the experimental case the agreement is accidental, since the measured gap is defined by excitonic states). The band structure obtained using the PBE optimized lattice constant of single-layer MoS$_2$ is shown in figure 2.

Hydrogenation leads to a significant modification of the band structure. We varied the number of H atoms from dilute...
Figure 10. The distribution of the hole (h) and electron (e) charges for the lowest energy excitonic states formed by different band charges: (a) top valence band (VB-h), two hydrogen (initially one occupied); (b) H-h and one empty; (c) H-e bands; and (d) bottom conduction band (CB) states for the 1/25 hydrogen density. The charge densities in (b) and (c) correspond to exciton C and those in (a) and (d) to exciton B defined in figure 8. The lateral dimensions of the super cell, X and Y, are in Å.

limit (1/25) to full coverage. For full hydrogen coverage, the system is in the metallic regime as evident from the band structure in figure 3(a) and the projected DOS are shown in figure 4(a). At low coverages (hydrogen concentrations 1/9 and 1/25) the system remains gapped and the electronic band structure includes partially-occupied spin-polarized mid gap states—occupied spin-up states and empty spin-down states (figure 5). These spin-polarized states are present in the dilute limit of the hydrogen concentration and are stable at least up to concentration ~10%. In the case of fully hydrogenated MoS$_2$, the system is in a paramagnetic metallic state. One can give the following reasoning for the above differences in the spin polarizations of the systems. While in the unpolarized case of full coverage the hydrogen atoms adsorb ‘vertically’ on S atoms, for partial H coverage, the angle between the H–S bond and MoS$_2$ plane is smaller than 90 degrees (tilted H–S bonds, see figure 1(c)). This difference in bonding results in different spin-state occupancies. Namely, for full-coverage the H 1s- and S 2p$_z$-states involved in the bonding and antibonding hybridized levels include only the $z$-components of the orbitals, while in the tilted case the hybridized states include also $p_x$ and $p_y$ orbitals of the sulfur atoms. As a result, there is a lower contribution of $z$-component of the orbital momentum of the H–S subsystem in the partially-covered case as compared to that of full coverage. Such a decrease of the orbital momentum of the H–S subsystem is compensated by an increase of its spin, i.e. in the partially covered system one obtains hydrogen states with a finite spin.

We have also performed corresponding calculations with adsorbed Li and Na atoms and found the systems to be in a paramagnetic metallic state at all values of adatom concentration (see figures 3(b), (c), 6(a) and (b), and also references [11,41]). A possible reason for this is the larger radius of the s-orbitals of Li and Na that is responsible for stronger hybridization of these states with those of MoS$_2$, and hence their delocalization, and diminished effects of spin-polarization.

3.2. Binding energies of excitons

In the pristine system, excitons are formed by conduction-band electrons and valence-band holes (figure 7). The excitonic binding energy ~1.067 eV obtained with the Slater XC kernel is of the same order of magnitude (albeit 2 times larger) when
compared with experimental data (0.22–0.57 eV) [40,42]. In the case of hydrogenated systems, the variety of excitonic states is much richer. As shown schematically in figure 8, one may expect bound states of electrons and holes formed by both MoS$_2$ and hydrogen bands. Solving equation (1) for the combinations of electron and hole bands in figure 8, we find that the corresponding binding energies are noteworthy, especially for the lower (1/25) coverage (see table 1).

Smaller binding energies of the ‘standard’ B exciton for the higher (1/9) coverage can be traced to enhanced screening effects arising from H electrons, and smaller binding energy of the hydrogen-state exciton, i.e. by hybridization of the ‘excitonic’ hydrogen states with those of the surrounding H atoms resulting in weakened electron-hole interaction. The strongest binding energy and the strength (i.e. probability of the transition to the corresponding exciton state, defined by equation (4)) was found for the C exciton, in which both electron and hole are localized on hydrogen atoms. This can be related to the local character of the charges that form the exciton. As mentioned above, the strength of this state decreases with increasing coverage. Another important result is the enhanced strength of the mixed excitonic states A and B at 1/9-coverage due to larger hybridization of the hydrogen and MoS$_2$ states at higher coverages (when the hydrogen electrons are more spread out over the surface).

3.3. Absorption and emission spectra

In figure 9, we plot the absorption and emission spectra for the pure and the 1/25 hydrogenated MoS$_2$ in the two-band approximation, as obtained using both DFT and TDDFT (Slater XC kernel), to highlight the difference. (In the hydrogenated case, the bands are the occupied and unoccupied mid-gap hydrogen bands.)

As expected the DFT optical spectra (figure 9) does not account for the presence of excitons, because of deficiencies in DFT with regard to exchange-correlation effects and because it is a theory suitable mainly for the system in its ground state. Both absorption and emission spectra are missing the excitonic contribution. What is more important here is that the emission spectrum of the hydrogenated system is in the infra-red frequency range (the peak of the spectrum is at ∼0.15 eV), while in the pristine system it is in the visible range (taking into account the fact that the DFT electronic bandgap 1.78 eV is ∼1 eV smaller than the experimental one [40]). The quench of the visible photoluminescence in single-layer MoS$_2$ after hydrogenation is in agreement with experimental observations [16].

3.4. Exciton charge distribution

For visualization of the size of the excitonic states, we have calculated charge distributions for the electron and hole states that form the valence-conduction and hydrogen-band excitons B and C (the ‘standard’ and the strongest-bound excitons, see figure 8) at different coverages. The results shown in figure 10 find the size of the excitons to be several angstroms for both cases. Importantly, the electron and hole that form the hydrogen-band exciton are not localized on the same atom (figure 10(a) and (b)).

4. Conclusions

We have studied electronic and excitonic properties of hydrogenated single-layer MoS$_2$, at three coverages, using a combined DFT and TDDFT approach. Our calculations show that for partial hydrogen coverage the system acquires spin-polarized mid gap states, and at full coverage transforms into a paramagnetic metal. The situation is very different with other s-orbital adsorbates—Li and Na—which produce a metallic regime at all coverages. We trace the difference in behavior to a weaker hybridization of H electrons with each other and MoS$_2$ states, owing to the smaller radius of the H-s wave function, compared to those of Li and Na, which produces localized mid-gap hydrogen states (flat bands).

We have further demonstrated that these spin-polarized states play a very important role in the absorption and excitonic properties of the system, resulting in a dominating hydrogen excitonic state with infrared absorption and emission, in contrast to the visible spectra exhibited by pure MoS$_2$. This result is in agreement with experimental data [16]. The existence of a mid-gap excitonic state in a hydrogenated 2D TMDC which has relatively large binding energy and long lifetime (large dipole strength) is an important finding by itself, one that may have applications in energy harvesting technologies.

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