Optoelectronic Properties of Rectangular Graphene Quantum Dots: Pariser-Parr-Pople Model Based Computational Study

Deepak Kumar Rai\textsuperscript{1} and Alok Shukla\textsuperscript{1,2}

\textsuperscript{1}Department of Physics, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India
\textsuperscript{2}Present Address: Department of Physics, School of Engineering and Applied Sciences, Bennett University, Plot No. 8-11, TechZone II, Greater Noida 201310, Uttar Pradesh, India

In this paper, we perform large-scale electron-correlated calculations of optoelectronic properties of rectangular graphene quantum dots (RGQDs) containing up to 56 carbon atoms. We consider the influence of increasing the length of RGQDs both along the zigzag, as well as arm-chair, directions on their optical properties. Theoretical methodology employed in this work is based upon Pariser-Parr-Pople (PPP) $\pi$-electron model Hamiltonian, which includes long-range electron-electron interactions. Electron-correlation effects were incorporated using multi-reference singles-doubles configuration-interaction (MRSDCI) method, and the ground and excited state wave functions thus obtained were employed to calculate the linear optical absorption spectra of the RGQDs, within the electric-dipole approximation. Our results on optical absorption spectra are in very good agreement with the experimental ones wherever available, for the hydrocarbon molecules with the same carbon-atom backbone structure as the RGQDs. In addition to the charge gap, spin gap of each quantum dot was also computed using the same methodology. Calculated spin gaps exhibit a decreasing trend with the increasing sizes of the RGQDs, suggesting that the infinite graphene has a vanishing spin gap. This result is consistent with the widespread belief that electron-correlation effects in graphene are weak.
I. INTRODUCTION

Despite many attractive properties, graphene has still not found applications in opto-electronic devices, because of the lack of a band gap. Therefore, in recent times, considerable amount of research effort has been directed towards graphene nanostructures such as quantum dots,$^{1,2}$ and nanoribbons,$^3$ which are expected to have band gaps because of quantum confinement. The idealized graphene nanoribbons (GNRs) have either zigzag or armchair edges, with substantially different electronic structure, and related properties. Theoretical studies reveal that zigzag GNRs (ZGNRs) exhibit edge magnetism with possible applications in spintronic devices,$^{4,5}$ while the armchair GNRs (AGNRs) are direct bandgap semiconductors, with potential optoelectronic applications.$^6,7$ If we consider either an AGNR or a ZGNR of a given width, and hypothetically cut it at two places perpendicular to its width the resultant rectangular structure, referred to as a rectangular graphene quantum dot (RGQD) will have both armchair and zigzag type edges. In this work we perform a computational study of optoelectronic properties of RGQDs, with the aim of understanding as to how they are influenced by the edge structure. Because the electronic properties of ZGNRs and AGNRs are very different from each other, it is of considerable interest as to how the electronic properties of RGQDs, which have both zigzag and armchair edges, evolve with the edge lengths. Such an understanding will help us in tuning the optoelectronic properties of RGQDs by manipulating their edges.

In our theoretical approach we consider graphene quantum dots to be systems whose low-lying excited states are determined exclusively by their $\pi$ electrons, with negligible influence of $\sigma$ electrons. As a result we adopt a computational methodology based upon the Pariser-Parr-Pople (PPP) $\pi$-electron Hamiltonian,$^8,9$ and configuration interaction (CI) approach employed in several of our earlier works on conjugated polymers,$^{10–16}$ and graphene quantum dots.$^{17–19}$ We adopt this approach to study RGQDs with the number of carbon atoms ranging from 28 to 56, corresponding to structures with increasing edge lengths in both armchair, and zigzag, directions. We further assume that the dangling carbon bonds at the edges are passivated by hydrogen, thus preventing edge reconstruction, and allowing the RGQDs to retain their symmetric shapes. As a matter of fact, these H-passivated RGQDs correspond to aromatic hydrocarbon molecules, for most of which experimental optical absorption data exists. Adopting the notation that RGQD-$n$ denotes a rectangular graphene quantum dot with $n$ carbon atoms, the chemical analogs of RGQD-28, -30, -36, -40, -42, -50, and -56 are aromatic compounds bisanthenes, terrylene, tetrabenzo coronene, quatterylene, teranthene, pentarylene and quateranthene, respectively. On comparing our theoretical results to the measured ones on these molecules, we obtain excellent agreement, thus validating our methodology.

Additionally, using the same MRSDCI methodology, we computed the spin gap of each RGQD studied in this work. We find that with the increasing sizes of the RGQDs, their spin gaps are decreasing, suggesting that the spin gap of infinite graphene vanishes.

Remainder of the paper is organized as follows. In the next section we briefly outline the theoretical methodology, while in section III we present and discuss our results. Finally, in section IV we present summary and conclusions.

II. STRUCTURE AND SYMMETRY

The schematic diagrams of RGQDs considered in this work are shown in Fig. 1. We have assumed that the dangling bonds on the edges of the quantum dots considered have been saturated by hydrogen atoms. Thus, the quantum dots considered here can be treated as planar hydrocarbons, exhibiting $\pi$ conjugation. We have assumed that all the quantum dots lie in the $xy$ plane, with idealized bond lengths of 1.40 Å, and bond angles of 120°.
Figure 1: Schematic diagrams of RGQDs considered in this work. For all the quantum dots, edge carbon atoms are assumed passivated by hydrogen. Notation RGQD-\(n\) denotes a rectangular graphene quantum dot with \(n\) carbon atoms.

Within the PPP model based theoretical methodology adopted here, small variations in bond lengths and angles do not make any significant differences to the calculated optical properties of such structures, as demonstrated by us earlier\(^{14,15}\). Having assumed the idealized geometry for the RGQDs, their point group symmetry is \(D_{2h}\), as in case of polyacenes studied by us earlier\(^{13-16}\). Because all the systems considered here have an even number of electrons, their ground state is of \(^1A_g\) symmetry, so that their one-photon dipole-connected excited states will be of the symmetries: (a) \(^1B_{3u}\), accessible by absorbing an \(x\)-polarized photon, and (b) \(^1B_{2u}\), reached through the absorption of a \(y\)-polarized photon.
III. THEORETICAL APPROACH

As discussed in the previous section, with hydrogen passivated edges, the quantum dots considered here are π-conjugated systems, and, therefore, in this work we employed Pariser-Parr-Pople (PPP) effective π-electron model Hamiltonian.\(^8\),\(^9\)

\[
H = -\sum_{i,j,\sigma} t_{ij} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i<j} V_{ij}(n_i - 1)(n_j - 1),
\]

where \(c_{i\sigma}^\dagger (c_{i\sigma})\) are creation (annihilation) operators corresponding to the \(p_z\) orbital of spin \(\sigma\), located on the \(i\)-th carbon atom, while the total number of electrons on the atom is indicated by the corresponding number operator \(n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}\). The first term in Eq. 1 denotes the one-electron hopping processes connecting \(i\)-th and \(j\)-th atoms, quantified by matrix elements \(t_{ij}\). We assume that the hopping connects only the nearest-neighbor carbon atoms, with the matrix element \(t_0 = 2.4\text{ eV}\), consistent with our earlier calculations on conjugated polymers,\(^10\)\(^-\)\(^16\) polyanromatic hydrocarbons,\(^20\),\(^21\) and graphene quantum dots.\(^18\),\(^19\) The second and the third terms in Eq. 1 represent the electron-electron repulsion terms, with the parameters \(U\), and \(V_{ij}\), representing the on-site, and the long-range Coulomb interactions, respectively. The distance-dependence of parameters \(V_{ij}\) is assumed as per Ohno relationship\(^22\)

\[
V_{ij} = U/\kappa_{i,j}(1 + 0.6117R_{ij}^2)^{1/2},
\]

where \(\kappa_{i,j}\) is the dielectric constant of the system, included to take into account the screening effects, and \(R_{i,j}\) is the distance (in Å) between the \(i\)th and \(j\)th carbon atoms. In the present set of calculations we have used two sets of Coulomb parameters: (a) the “screened parameters”\(^23\) with \(U = 8.0\text{ eV}\), \(\kappa_{i,j} = 2.0(i \neq j)\), and \(\kappa_{i,i} = 1.0\), and (b) the “standard parameters” with \(U = 11.13\text{ eV}\) and \(\kappa_{i,j} = 1.0\).

We initiate the computations by performing restricted Hartree-Fock (RHF) calculations for the closed-shell singlet ground states of the RGQDs considered here, by employing the PPP Hamiltonian (Eq. 1), using a computer program developed in our group.\(^24\) The molecular orbitals (MOs) obtained from the RHF calculations are used to transform the PPP Hamiltonian from the site representation, to the MO representation, for the purpose of performing many-body calculations using the CI approach. The correlated-electron multi-reference singles-doubles configuration interaction (MRSDCI) approach was employed in this work, which consists of a CI expansion obtained by exciting up to two electrons, from a chosen list of reference configurations, to the unoccupied MOs.\(^25,\)\(^26\) The reference configurations included in the MRSDCI method depend upon the targeted states, which can be ground state or one-photon excited states. In all the CI calculations, only the configurations consistent with the spin and point group symmetries of the targeted states are included. Nevertheless, in cases of larger dots namely RGQD-50, -54, and -56, we had to resort to the frozen orbital approximation to keep the CI expansion tractable. This consists of freezing a few lowest energy occupied MOs, and removing the corresponding charge-conjugation symmetric virtual MOs from the list, as described in our earlier works.\(^14,\)\(^15,\)\(^18\)

Once CI calculations are finished, the many-body wave functions obtained are used to compute the transition electric dipole matrix elements connecting one-photon excited states to the ground state. The transition dipole elements, along with the excitation energies of the excited states, are used to compute the optical absorption cross-section \(\sigma(\omega)\), according to the formula

\[
\sigma(\omega) = 4\pi\alpha \sum_i \frac{\omega_i |\langle i|\epsilon \cdot r|0\rangle|^2 \gamma^2}{(\omega_i - \omega)^2 + \gamma^2}.
\]

In the equation above, \(\omega\) denotes frequency of the incident light, \(\epsilon\) represents its polarization direction, \(r\) is the position operator, \(\alpha\) denotes the fine structure constant, indices \(0\) and \(i\) represent, respectively, the ground and excited states, \(\omega_i\) is the frequency difference between those states, and \(\gamma\) is the assumed universal line width. The summation over \(i\), in principle, is over an infinite number of states which are dipole connected to the ground state. However, in practice, the sum includes only those excited states whose excitation energies are within a certain cutoff, normally taken to be 8 eV.

IV. RESULTS AND DISCUSSION

In order to assess the role played by electron-correlation effects on various properties of RGQDs, it is important first to understand the independent particle results obtained using the tight-binding (TB) model. Therefore, in this section, we first present the result obtained by TB model, followed by those obtained by the PPP-model.
A. Tight-Binding Model Results

1. Electron Density

Here, we present the electron density associated with the edge atoms, for the highest occupied molecular orbital (HOMO), and the lowest unoccupied molecular orbital (LUMO), for various GQDs, as a function of their size. The reason we choose only HOMO and LUMO is because these orbitals are involved in the first absorption peak of all the RGQDs, thus determining their low-energy optical properties. The electron density corresponding to the edge atoms, for the $i$-th orbitals is defined as

$$\rho_{\text{edge}}^{(i)} = \sum_{\mu \in \text{edge}} |C_{\mu i}|^2$$

where, $\mu$ denotes an atomic site, $C_{\mu i}$ is the corresponding MO coefficient, and the “edge” refers either to the armchair edge, or the zigzag edge. Because of the electron-hole symmetry in the nearest-neighbor TB-model, the magnitude of the MO coefficients $C_{\mu i}$ in HOMO and LUMO is the same, so that $\rho_{\text{edge}}^H = \rho_{\text{edge}}^L$, where superscripts $H(L)$ imply HOMO(LUMO) orbitals. Thus, in the following we refer to a corresponding electron density as $\rho_{\text{edge}}^{H/L}$, and study it as a function of the size of RGQDs. In order to examine electron densities as a function of dimensions of RGQDs, we use two width parameters $N_z$ and $N_a$, which are normally utilized for quantifying the widths of graphene nanoribbons. $N_z$ denotes the number of zigzag lines in the RGQD across the armchair edge, and thus quantifies the length of the armchair edge. Similarly, $N_a$ denotes the number of dimer lines across the zigzag edge, thus representing the length of the zigzag edge. Therefore, if we denote the dimensions of a given RGQD using the notation $N_a \times N_z$, RGQD-40 (Fig. 1b) will be denoted as $5 \times 8$, and RGQD-54 (Fig. 1h) can be represented as $9 \times 6$. Noteworthy point is that the product of $N_a$ and $N_z$ is nothing but the total number of carbon atoms $n$ in the quantum dot.

From the definitions of $N_a$ and $N_z$ it is obvious that, when the length of the quantum dot is increased in the zigzag direction holding its width fixed, it corresponds to a fixed value of $N_z$, and increasing values of $N_a$. Similarly, increasing length of the quantum dot in armchair direction, for the fixed width implies that $N_a$ is fixed, while $N_z$ is increasing. Behavior of $\rho_{\text{edge}}^{H/L}$, both for armchair and zigzag edges, for increasing lengths of RGQDs, for various widths is shown in 2. From Fig. 2(a) it is obvious that for a given width, with the increasing zigzag length, $\rho_{\text{edge}}^{H/L}$ resides mostly on the zigzag edges, as compare to the armchair ones. From Fig. 2(b), for various widths and increasing lengths in the armchair directions, the following trends emerge: (a) The value of $\rho_{\text{edge}}^{H/L}$ on armchair edges increases towards saturation for a given width, (b) the electron density on the zigzag edges decreases towards saturation for a given width, (c) for $N_a = 5$, the saturated value of the electron density of the zigzag edge is less than that on the armchair edge, however, the trend reverses for $N_a = 7$ and $N_a = 7$. Thus, we conclude that for sufficiently wide RGQDs, the tendency of the electron density of the HOMO-LUMO orbitals is to accumulate on the zigzag edges. Therefore, we conclude that impurity substitution on the zigzag edges can be efficiently use to tune the optoelectronic properties of RGQDs.
2. Energy Levels

In this section, we present and discuss the behavior of the energy levels and the optical gap, with the increasing sizes of RGQDs. In Fig. 3, we have presented the energy level diagrams for RGQDs of varying sizes. The energy level diagrams are arranged in such a manner that if we move from left to right \( N_z \) increases, while \( N_a \) is fixed. On examining these, we observe the following trends: (a) The electron and hole levels are mirror symmetric with respect to the Fermi level \( (E = 0) \), as a consequence of the electron-hole symmetry of the nearest neighbor tight-binding model, (b) the lack of any energy level at \( E = 0 \) for any of the RGQDs is consistent with the vanishing density of states at the Fermi level, for infinite graphene.
3. Linear Optical Absorption Spectra and Optical Gaps

In Fig. 4, we have presented optical absorption spectra of RGQDs of varying sizes computed using the TB model. The following conclusions can be drawn from this graph:

1. The first peak in the absorption spectra for all the RGQDs is $y-$polarized, and corresponds to excitation of an electron from HOMO to LUMO, leading to the excited state $1^1B_{2u}$. Therefore, this peak corresponds to the optical gap of the concerned RGQDs, and it is the most intense peak in the spectra.

2. The intensity of the first peak in the spectra increases significantly with the increasing size of RGQDs.

3. We also note that all $y-$polarized peaks are non-degenerate, and correspond to excited states of symmetry $1B_{2u}$, as per the selection rules of $D_{2h}$ point group. All $x-$polarized peaks are doubly degenerate, as a consequence of electron-hole symmetry of the nearest neighbor TB model, and correspond to excited states of $1B_{3u}$ symmetry. For example, in RGQD-30, first peak is $y-$polarized, and it is due to non-degenerate excitation $|H \rightarrow L\rangle$, while the second peak is $x-$polarized, and is due to doubly degenerate excitations $|H \rightarrow L + 3\rangle$ and $|H - 3 \rightarrow L\rangle$. As mentioned earlier, notations $H/L$ imply HOMO/LUMO. Similarly, notations $H - m (L + n)$ imply $m$-th orbital below HOMO ($n$-th orbital above LUMO).

4. With the increasing length of the RGQDs along a given orientation (zigzag or armchair), the optical gap decreases.
Next, we investigate the nature of optical gap of RGQDs as a function of their size. The optical gaps for various widths, and increasing lengths of RGQDs are presented in Fig. 5, from which it is obvious that for a given width, band gaps of all the RGQDs decrease towards zero, with the increasing lengths. The rate of decrease of the gap with increasing length is faster for ribbons of the larger widths. It is also obvious that for a given length, the gaps decrease with the increasing widths.

Figure 4: Linear optical absorption spectra for RGQDs, computed using the TB model. The spectrum has been broadened with a uniform line-width of 0.1 eV.
In Table I, we compare the HOMO-LUMO gap obtained at the tight-binding level, with the experimental results, wherever available. For the sake of comparison, we also present the values of optical gaps obtained using the PPP-CI approach to be discussed in the next section. From the table it is obvious that the gaps obtained using the TB model are much smaller than the experimental values. On the other hand, the PPP-CI values of the optical gaps, are generally in much better agreement with the experiments. Therefore, it is obvious that the TB model cannot provide good quantitative agreement with the experiments, because it ignores the electron-correlation effects.
Table I: Optical gaps of various RGQDs obtained using the TB model, and the PPP model. In case of PPP model, the gaps are computed using the CI approach, by employing both the screened and the standard parameters, denoted below as SCR, and STD, respectively.

| System   | optical gap (eV)          |                |                |
|----------|---------------------------|----------------|----------------|
|          | TB Model                  | PPP-CI         | Experimental   |
|          | SCR | STD |                   |                |
| RGQD-28  | 0.85 | 2.00 | 2.21              | 1.80,28, 2.02,29, 2.1529 |
| RGQD-30  | 1.16 | 2.11 | 2.43              | 2.14,31, 2.21,35,36, 2.2234 |
| RGQD-36  | 0.45 | 2.11 | 2.30              | -              |
| RGQD-40  | 0.89 | 2.02 | 2.30              | 1.84,38, 1.87,32,34, 1.9139 |
| RGQD-42  | 0.44 | 1.86 | 2.04              | -              |
| RGQD-50  | 0.72 | 1.72 | 1.98              | 1.6632,34      |
| RGQD-54  | 0.17 | 1.63 | 2.09              | -              |
| RGQD-56  | 0.24 | 1.50 | 1.91              | 1.3530         |

B. PPP Model Based CI Results

In this section, we present our results obtained from the PPP-model based CI calculations. First, we present the result on the spin gaps of different RGQDs, followed by their linear optical absorption spectra.

1. Spin Gaps

Spin gap of an electronic system is the energy difference between the lowest triplet and singlet states. For RGQDs, the lowest singlet state is $1^1A_g$ ground state, while the lowest triplet state is the $1^3B_{2u}$ state, whose spatial part of the wave function consists predominantly of the single excitation $|H \rightarrow L\rangle$, just as in the case of $1^1B_{2u}$ state. Thus, at the TB level, $1^1B_{2u}$ and $1^3B_{2u}$ will be degenerate, and, therefore their spin and optical gaps will be identical. However, if the two gaps are found to be different for RGQDs, it can only be due to electron-electron interactions. Therefore, difference in the spin and optical gaps is a measure of the electron correlation effects in RGQDs. With this in mind, we computed the spin gaps of all RGQDs studied in this work, using our PPP model based MRSDCI approach. Because, to compute the spin gaps we needed energies of $1^1A_g$ and $1^3B_{2u}$ states which are in different symmetry manifolds, we managed to perform very large-scale MRSDCI calculations, as is evident from Table II. Therefore, we believe that our results on spin gaps of RGQDs presented in Table III are fairly accurate. From the inspection of Table III it is obvious that spin gap of RGQDs is decreasing with their increasing sizes. Thus, this result suggests that the spin gap of infinite graphene is zero, consistent with the widespread assumption that graphene is a weakly-correlated material. It will also be interesting to compare the experimental values of the spin-gaps of individual hydrocarbon molecules corresponding to these RGQDs, with our calculated values. Therefore, we urge the experimentalists to measure the spin gaps of hydrogen passivated counterparts of various RGQDs studied in this work.
Table II: Dimensions of the CI matrices ($N_{total}$) for different symmetry subspaces, employed in the calculations of spin gaps of RGQDs containing $n$ carbon atoms.

| $n$ | $^1A_g$ | $^1B_{2u}$ |
|-----|---------|------------|
| 28  | 1630819 | 3363548    |
| 30  | 929383  | 2052250    |
| 36  | 1271636 | 2516476    |
| 30  | 1355882 | 2224033    |
| 36  | 2895688 | 6999314    |
| 30  | 3470683 | 8213570    |
| 40  | 5346813 | 9103538    |
| 42  | 4690547 | 8964411    |
| 42  | 5694171 | 10937480   |
| 50  | 3504598 | 3371187    |
| 54  | 2655705 | 5103671    |
| 56  | 4170514 | 10745638   |
| 56  | 3945223 | 9939690    |
| 56  | 5913511 | 10766994   |
| 56  | 4181480 | 9476458    |

MRSDCI<sup>a</sup> method with screened parameters.
MRSDCI<sup>b</sup> method with standard parameters.

Table III: Singlet-Triplet gaps ($\Delta E_{ST} = E(1^3B_{2u}) - E(1^1A_g)$) of RGQDs, computed using the MRSDCI method, employing screened (Scr) and standard parameters (Std) in the PPP model. RGQDs are divided in groups of three, where each group corresponds to a common width, and increasing armchair length.

| System | $\Delta E_{ST}$ (eV) |
|--------|----------------------|
|        | Scr      | Std     |
| RGQD-30| 1.11     | 1.30    |
| RGQD-40| 0.97     | 1.16    |
| RGQD-50| 0.79     | 0.94    |
| RGQD-28| 0.76     | 0.75    |
| RGQD-42| 0.40     | 0.36    |
| RGQD-56| 0.15     | 0.11    |
| RGQD-36| 0.37     | 0.34    |
| RGQD-54| 0.13     | 0.07    |
| RGQD-72| 0.05     | 0.02    |

2. Linear optical absorption spectrum

In this section, we present optical absorption spectra of RGQD-$n$, with $n$ ranging from 30 to 56, computed using the PPP model, and the MRSDCI approach. Before discussing the results of our calculations, in Table IV we give the sizes of the CI matrices, for different symmetry spaces of various RGQDs. The fact that the sizes of the CI matrices were in the range $2.43 \times 10^5 - 6.19 \times 10^6$, implies that these calculations were indeed large scale, and, therefore, should be fairly accurate. For RGQD-$n$, $n = 28$ to 42, all the $n$ MO’s of the systems were included in the MRSDCI calculations. However, from $n = 50$ to 56, it was no longer possible to perform accurate calculations with all the $n$ orbitals. Therefore, for these cases, some low-lying occupied MO’s, were frozen, while their unoccupied counterparts were deleted.
Table IV: Dimension of the CI matrices ($N_{\text{total}}$) of different symmetry subspaces involved in the MRSDCI calculations of the optical absorption spectra of various RGQDs.

| $n$ | $^1A_g$ | $^1B_{2u}$ | $^1B_{3u}$ |
|-----|---------|------------|------------|
|     | $N_{\text{total}}$ | $N_{\text{total}}$ | $N_{\text{total}}$ |
| 28  | 243473$^a$ | 1286950$^a$ | 1195300$^a$ |
| 176670$^a$ | 1304940$^a$ | 1363812$^a$ |
| 30  | 148576$^a$ | 1417769$^a$ | 1128568$^a$ |
| 210078$^a$ | 1650565$^a$ | 1229074$^a$ |
| 36  | 1093085$^a$ | 1309198$^a$ | 1506432$^a$ |
| 1149578$^a$ | 1983952$^a$ | 1607780$^a$ |
| 40  | 2675017$^a$ | 4768452$^a$ | 3136672$^a$ |
| 3807268$^a$ | 6200883$^a$ | 4820202$^a$ |
| 42  | 2729332$^a$ | 3551497$^a$ | 3195172$^a$ |
| 3477479$^a$ | 395229$^a$ | 4042750$^a$ |
| 50  | 3504598$^a$ | 4494916$^a$ | 5083760$^a$ |
| 2655705$^a$ | 5637511$^a$ | 6193064$^a$ |
| 54  | 2150043$^a$ | 2473193$^a$ | 3038570$^a$ |
| 3047218$^a$ | 4003216$^a$ | 357911$^a$ |
| 56  | 2125583$^a$ | 2983416$^a$ | 3013058$^a$ |
| 2830899$^a$ | 3086912$^a$ | 3308186$^a$ |

MRSDCI$^a$ method with screened parameters.  
MRSDCI$^b$ method with standard parameters.

The calculated spectra of these RGQDs are presented in Fig. 6, while the important information regarding the excited states contributing to various peaks in the spectra are presented in Tables I-XVI of Supporting Information.
Figure 6: Computed linear optical absorption spectra of RGQDs, obtained using the MRSDCI approach: (a) by employing screened Coulomb parameters in the PPP model, (b) by employing standard Coulomb parameters in the PPP model. In both the cases, the spectra have been broadened using a uniform line-width of 0.1 eV.
Before discussing the spectra of individual RGQDs, we discuss the general trends observed in our calculation:

1. For each RGQD-\( n \), the absorption spectrum obtained using the PPP-CI approach is blueshifted in comparison to the TB model.

2. For all the RGQDs, absorption spectra obtained using the screened parameters are red-shifted compared to those obtained using the standard parameters.

3. In all cases, the first peak of the spectrum is due to optical excitation from the \( 1^1 A_g \) ground state to \( 1^1 B_{2u} \) excited state, and corresponds to the optical gap. As per electric dipole selection rules, this peak is \( y \)-polarized.

4. For all the RGQDs, the first peak is not the most intense peak. For a number of RGQDs, several high energy peaks are more intense than the first one. This result is in sharp contrast with the TB model results.

5. Dominant configurations in the wave functions of the excited states corresponding to the lower energy peaks are single excitations, while those in the higher energy peaks are dominated by double and higher excitations.

A comparison of calculated peak positions with the experimentally measured values, and the theoretical results of other authors, for RGQD-28, RGQD-30, RGQD-36, RGQD-40, RGQD-42, RGQD-50 and RGQD-56 is presented in Tables V, VI, VII, VIII, IX, X, and XII, respectively. For RGQD-54, we could not locate any previous experimental or theoretical data.

**RGQD-28**

Clar and Schmidt,\(^{29}\) Arabei \textit{et al.},\(^{30}\) and Konishi \textit{et al.}\(^{28}\) have reported the measurements of the absorption spectrum of bisanthenes, and its derivatives, the structural analogs of RGQD-28. In Fig. 6 (a) and (b), we present our calculated spectra using the screened and standard parameters, respectively, within the PPP-CI approach. If we compare the relative intensity of the first peak of the experimental spectra, we find that results of Arabei \textit{et al.}\(^{30}\) are in perfect agreement with our results in that the first peak is not the most intense. However, Konishi \textit{et al.}\(^{28}\) report that the first peak is the most intense one, in complete disagreement with our results. Our calculated location of the first peak corresponding to the optical gap, was found to be 2.00 eV with the screened parameters, and 2.21 eV for the standard parameters. As is obvious from Table V, the experimental values of the optical gap range from 1.80 eV to 2.15 eV. Thus, we find that both our screened and standard parameter of optical gap are quite close to the range of experimental values. We also note that our screened parameter of 2.00 eV is in almost perfect agreement with the value of optical gap 2.02 eV, measured by Clar and Schmidt.\(^{29}\) As far as higher energy peaks are concerned, Arabei \textit{et al.} report a peak at 2.43 eV for which there are no counterparts in our calculated spectra. Konishi \textit{et al.}\(^{28}\) measured a peak at 3.64 eV, while Arabei \textit{et al.}\(^{30}\) measured one at 3.87 eV. Comparing our calculations to these, we find there is no matching peak at 3.64 eV; however, our screened parameters spectrum has a peak at 3.87 eV, in perfect agreement with Arabei \textit{et al.}\(^{30}\). Next experimental peak located at 4.05 eV, reported by Konishi \textit{et al.},\(^{28}\) is in good agreement with our standard parameter peak computed at 4.14 eV, while the corresponding screened parameter candidate at 4.19 eV is somewhat higher. The highest measured peak located at 4.80 eV, reported by Arabei \textit{et al.}\(^{30}\) is in reasonable agreement with the standard parameter value of 4.68 eV, while screened parameter value of 4.49 eV is significantly smaller. Furthermore, we have computed several higher energy peaks as well, for which no experimental results exist. We hope that in future measurements of the absorption spectrum of bisanthenes, energy range of 5 eV, and beyond, will be explored.

On comparing our results to calculations by other authors, we find that the TDDFT value of the optical gap computed by Malloci \textit{et al.}\(^{41}\) is significantly smaller than our results, as well as experiments. However, Parac and Grimme\(^{42}\) report a TDDFT value of the optical gap at 1.78 eV, which is in very good agreement with the lowest measured experiment value of the optical gap, 1.80 eV.\(^{28}\) They also report a TDPPP value of the optical gap which is in very good agreement with our screened parameter result, as well as other experimental results. As far as higher energy peaks computed by Malloci \textit{et al.} are concerned, our PPP model values are generally in good agreement with them.

The many-particle wave function of the \( 1B_{2u} \) state corresponding to the optical gap is dominated by the single excitation \( |H \rightarrow L\rangle \), where \( H \) and \( L \), respectively, denote the HOMO and the LUMO of the system. Peak VI is the most intense peak in the absorption spectra computed using both the screened as well as the standard parameters. The most intense peak computed using the screened parameters located at 5.63 eV, corresponds to a state with \( B_{3u} \) symmetry, whose wave function is dominated by \( |H-2 \rightarrow L + 4\rangle \)-\textit{c.c.} excitations, where \textit{c.c.} denotes the charge conjugated configuration. However, the standard parameter calculations predict the most intense intense peak to be due to a \( B_{3u} \) state, located at 5.95 eV, along with a small mixture of a \( B_{2u} \) state located at 6.17 eV, with their wave
functions dominated by single excitations $|H→L+ 4⟩−\text{c.c.}$, and $|H→L+ 3⟩$, respectively. The detailed wave function analysis of all the excited states contributing to various peaks in the calculated spectra of RGQD-28, is presented in Tables I and II of the Supporting Information.

Table V: Comparison of calculated peak locations in the optical absorption spectra of RGQD-28, with the experimental, and other theoretical results, for bisanthen. The calculations were performed using the PPP-MRSDCI approach, employing both the screened and the standard parameters. All results are in eV units.

| Experiments | Theory (others) | This work |
|-------------|-----------------|-----------|
|             | Screened        | Standard  |
| 1.80, 2.02, 2.15, 3.64, 3.87, 4.05, 4.80 | 1.47, 1.78, 1.98 | 2.00 ($^1B_{2u}$), 2.21 ($^1B_{2u}$) |
| -            | 2.83, 2.96     | -         |
| 3.64, 3.87, 4.05, 4.80 | 3.76, 5.39, 4.35 | 3.87 ($^1B_{3u}$), 5.22 ($^1B_{2u}$), 6.35 ($^1B_{3u}$) |
| -            | -               | -         |
| 4.05, 4.77   | 4.19, 4.49, 5.63 | 4.14 ($^1B_{3u}$), 6.05 ($^1B_{2u}$) |
| -            | -               | 5.09 ($^1B_{3u}$) |
| 4.80, 5.91   | 4.49, 5.22      | 4.68 ($^1B_{3u}$), 5.41 ($^1B_{2u}$) |
| -            | -               | 6.06 ($^1B_{2u}$) |
| -            | 6.35           | 6.41 ($^1B_{2u}$) |
| -            | -               | -         |
| 7.09         | 7.03           | 6.80 ($^1B_{2u}$) |

Koch et al., Ruiterkamp et al., and Halasinski et al. have reported the measurements of the absorption spectrum of terylene, the structural analog of RGQD-30, and its derivatives. However, Clar et al., Kummer et al., Biktchantaev et al. and Baumgarten et al. reported only the optical gap of terylene. In Fig. 6 (a) and (b), we present our calculated spectra using the screened and standard parameters, respectively, within the PPP-CI approach. If we compare the relative intensity of the first peak of the experimental spectra, we find that the results of Koch et al., Ruiterkamp et al. and Halasinski et al. are in perfect agreement with our results in that the first peak is not the most intense. The calculated location of the first peak of the absorption spectrum, which defines the optical gap, was found to be 2.11 eV, and 2.43 eV, from our standard, and screened parameter based calculations, respectively. As it is obvious from Table VI, that the experimental values of the optical gap range from 2.14 eV to 2.36 eV. Thus, we find that both our screened and standard parameter of optical gap are quite close to the range of experimental values. We also note that our screened parameter value of 2.11 eV is in almost perfect agreement with the value of optical gap 2.14 eV, measured by Kummer et al. As far as higher energy peaks are concerned, we have a peak at 4.07 eV from our screened parameter calculations, for which there are no available counterparts in the experiments, or the theoretical works of other authors. Halasinski et al. measured a peak at 4.33 eV, close to which our calculations predict no peak. However, Koch et al. measured a peak at 4.47 eV, which is in good agreement with a peak at 4.58 eV, predicted by our screened parameter calculations. Next experimental peak located at 4.71 eV, reported by Halasinski et al. and Ruiterkamp et al., is in good agreement with our standard parameter peak computed at 4.75 eV. Koch et al., Ruiterkamp et al. and Halasinski et al. have also reported several higher peaks which are in reasonably good agreement with our computed screened and standard results. Furthermore, we have computed several higher energy peaks as well, for which no experimental results exist. We hope that in future measurements of the absorption spectrum of terylene, energy range of 7 eV and beyond will be explored.

On comparing our results to the theoretical works by other authors, we find that the value of the optical gap reported by Malloci et al., Minami et al. and Karabunarliev et al. are slightly larger than our screened parameter results. On the other hand, the gaps reported by Halasinski et al. and Viruela et al. are slightly smaller than our screened parameter results. As far as higher energy peaks computed by Malloci et al. are concerned, our PPP model values are generally in good agreement with them.

The many-particle wave function of the $1B_{2u}$ state corresponding to the optical gap is dominated, as expected, by the single excitation $|H→L⟩$. In the spectra computed using the screened parameters, IV peak is most intense, and it is due to a $B_{2u}$ state, located at 5.12 eV, whose wave function is dominated by the $|H→L+ 2⟩$ excitation. For the standard parameter calculations, peak V is the most intense one, due to a $B_{2u}$ state located at 6.01 eV, along with a small mixture of $B_{3u}$ state located at 5.87 eV, with wave functions dominated by configurations $|H→L+ 3⟩$, and $|H→L; H→L+ 4⟩−\text{c.c.}$, respectively. The detailed wave analysis of all the excited states contributing peaks in
Table VI: Comparison of calculated peak locations in the optical absorption spectra of RGQD-30, with the experimental, and other theoretical results, for terylene. The calculations were performed using the PPP-MRSDCI approach, employing both the screened and the standard parameters. All results are in eV units.

| Experiments | Theory (others) | This work |
|-------------|----------------|-----------|
|             |                | Screened  | Standard |
| -           | -              | 2.11 ($^1B_{2u}$) | 2.43 ($^1B_{2u}$) |
| -           | 4.71,34,35     | -         | 4.75 ($^1B_{3u}$) |
| 5.20,34,35  | -              | 5.12 ($^1B_{2u}$) | 5.03 ($^1B_{3u}$) |
| 5.41,34,35  | -              | 5.35 ($^1B_{3u}$) | 5.53 ($^1B_{2u}$/$^1B_{3u}$) |
| 6.10,34     | 6.19,37,34     | 6.08 ($^1B_{3u}$) | 6.01 ($^1B_{2u}$) |
| 6.44,34     | -              | 6.47 ($^1B_{3u}$) | 6.24 ($^1B_{3u}$) |
| 6.69,34     | 6.83           | 6.86 ($^1B_{3u}$) | 6.76 ($^1B_{3u}$) |

*TDDFT method, *DFT(Kohan-Sham) method

The hydrogen passivated structural analog of RGQD-36 is tetrabenzocoronene, for which we were unable to locate any experimentally measured optical absorption spectrum. Therefore, we can only compare our calculations to the theoretical works of other authors, for which also we could find just one TDDFT based computation of the optical absorption spectra by Malloci et al.47 In Fig. 6 (a) and (b), we present our calculated spectra using the screened and standard parameters, respectively, within the PPP-CI approach. If we compare the relative intensity of the first peak in the spectra, we find that the results of Malloci et al.47 are in perfect agreement with our results in that the first peak is not the most intense. In Table VII, we have compared the locations of various peaks reported by Malloci et al. with our computed results. We find that the value of optical gap reported by Malloci et al.43 is 0.95 eV, which significantly smaller than our computed results of 2.11 eV (screened) and 2.30 eV (standard). Given such severe disagreement between two theoretical calculations, it will be really useful if an experiment is performed on this molecule, or another theoretical calculation is done. Given the fact that our results on optical gaps on smaller RGQDs were in excellent agreement with the experiments, we speculate that the TDDFT calculation of Malloci et al.47 has significantly underestimated the optical gap of RGQD-36. As far as higher peaks are concerned Malloci et al.47 have report a peak at 3.16 eV, for which there is no counterparts is available in our computed spectra. Our next peak using screened parameter is located at 3.63 eV, which is in perfect agreement with the value 3.64 reported by Malloci et al.47 As far as higher energy peaks computed by Malloci et al.47 are concerned, our PPP model values are generally in good agreement with them.

The many-particle wave function of the $1B_{2u}$ state corresponding to the optical gap is dominated by the single excitation $|H \to L\rangle$, similar to the case of smaller RGQDs. For both the screened as well as the standard parameters computed absorption spectra, peak VIII is the most intense one. In the spectra computed using the screened parameters, the most intense peak is located at 5.99 eV, and is due to states of symmetries $B_{2u}$ and $B_{3u}$ contributing almost equally to the oscillator strength, with their many-particle wave functions dominated by configurations $|H - 3 \to L + 3\rangle$, and $|H - 2 \to L + 5\rangle + c.c.$, respectively. In the spectrum computed using the standard parameters, the most intense peak is located at 6.57 eV, due to a $B_{3u}$ state, with wave function dominated by $|H - 5 \to L + 2\rangle + c.c.$ excitations. The detailed wave analysis of excited states contributing peaks in the spectra computed by the screened, and the standard parameters is presented in Tables V and VI of the Supporting Information.
Table VII: Comparison of calculated peak locations in the optical absorption spectra of RGQD-36, with theoretical results of other authors for tetrabenzo coronene. No experimental results are available for this molecule. The calculations were performed using the PPP-MRSDCI approach, employing both the screened and the standard parameters. All results are in eV units.

| Theory (others) | This work |
|----------------|-----------|
|                | Screened  | Standard |
| 0.95           | -         | -        |
| -              | 2.11 (\(1B_{2u}\)) | 2.30 (\(1B_{2u}\)) |
| 3.16           | -         | -        |
| 3.64           | 3.63 (\(1B_{3u}\)) | -        |
| -              | 3.77 (\(1B_{2u}\)) | 3.87 (\(1B_{2u}\)) |
| -              | 4.01 (\(1B_{2u}/1B_{3u}\)) | -        |
| -              | 4.35 (\(1B_{2u}\)) | 4.41 (\(1B_{2u}/1B_{3u}\)) |
| 4.83           | 4.94 (\(1B_{3u}\)) | 4.88 (\(1B_{2u}\)) |
| -              | -         | 5.00 (\(1B_{3u}\)) |
| -              | 5.65 (\(1B_{2u}\)) | 5.60 (\(1B_{3u}\)) |
| -              | 5.99 (\(1B_{2u}/1B_{3u}\)) | 5.86 (\(1B_{2u}/1B_{3u}\)) |
| 6.22           | 6.50 (\(1B_{2u}\)) | 6.57 (\(1B_{2u}\)) |

Ruiterkamp et al., Koch et al., Halasinski et al. have reported the measurements of the absorption spectrum of quaterrylene, the hydrogen passivated structural analog of RGQD-40, and its derivatives. However, Clar et al., Former et al., Gudipati et al., and Baumgarten et al. reported only the optical gap ofquaterrylene. In Fig. 6 (a) and (b), we present our calculated spectra using the screened and the standard parameters, respectively, within the PPP-CI approach. If we compare the relative intensity of the first peak of the experimental spectra, we find that results of Ruiterkamp et al. and Halasinski et al. are in perfect agreement with our results in that the first peak is not the most intense. However, Koch et al. report that the first peak is the most intense one, in disagreement with our results, as well as those of other experimentalists. In Table VIII, we present the locations of important peaks obtained from our calculations, and compare them to the experimental results, as well as theoretical calculations of other authors. As is obvious from the table, the experimental values of the optical gap range from 1.87 eV to 2.04 eV, implying that our screened parameter result of optical gap (2.02 eV) is quite close to the range of experimental values, while the optical gap obtained using the standard parameters (2.30 eV) is somewhat larger. We also note that our screened parameter value of the optical gap, 2.02 eV, is in almost perfect agreement with 2.03 eV, the value of the optical measured by Clar and Schmidt. As far as the higher energy peaks are concerned, Koch et al. report peaks at 3.71 eV and 3.85 eV, Halasinski et al. report a peak at 3.78 eV, while Ruiterkamp et al. report one at 3.86 eV. Although, our calculated spectra have no peaks precisely at these locations, however, the screened parameters spectrum has a peak at 4.06 eV, in reasonable agreement with Ruiterkamp et al., and the higher energy peak of Koch et al. After that the experimental peaks located at 4.71 eV and 4.83 eV, reported by Halasinski et al., are in good agreement with our standard parameter peak computed at 4.85 eV. The next higher measured peaks reported by Koch et al. at 5.27 eV is in good agreement with our screened-parameter based peak at 5.16 eV. Halasinski et al. report a peak at 5.39 eV, which is in good agreement with the peak at 5.48 eV, predicted by standard parameter calculations. Furthermore, Halasinski et al. have measured four more peaks in the range 5.82 — 6.63 eV, each of which is in good agreement with our calculated peaks (see Table VIII).

On comparing our results to the calculations by other authors, we find that values of optical gap reported by Viruela et al., Halasinski et al., and Halasinski et al. are significantly smaller than our results as well as experiments. However, TDDFT calculations of Mallocci et al., Gudipati et al., and Minami et al., and PM3/CI results of Karabunarliev et al. are in reasonably good agreement with the experiment, and our calculated values, of the optical gaps. As far as higher energy peaks computed by Mallocci et al. and Minami et al. are concerned, our PPP model values are generally in good agreement with them.

The many-particle wave function of the \(1B_{2u}\) state corresponding to the optical gap is, quite expectedly, dominated by the single excitation \(|H \rightarrow L\). In the spectra computed using the screened parameters, peak IV is most intense, and it is due to a state of \(B_{2u}\) symmetry, located at 5.16 eV, along with a small contribution from a \(B_{3u}\) state, located at 5.17 eV. The wave functions of these states are dominated by single excitations \(|H \rightarrow L + 2\rangle\), and \(|H \rightarrow L + 1\rangle\) \(\rightarrow\text{c.c.}\), respectively. For the standard parameter calculations, peak VI is the most intense one, corresponding again to a mixture of a \(B_{2u}\) state (at 6.23 eV), and a \(B_{3u}\) state (at 6.17 eV), with wave functions dominated by excitations...
\(|H - 4 \rightarrow L + 4\rangle\), and \(|H \rightarrow L + 1; H - 6 \rightarrow L\rangle - c.c., respectively. The detailed wave function analysis of the excited states contributing to various peaks in the spectra calculated by the screened and standard parameters, respectively, is presented in Tables VII and VIII the Supporting Information.

Table VIII: Comparison of calculated peak locations in the optical absorption spectra of RGQD-40, with the experimental, and other theoretical results, for quaterpylene. The calculations were performed using the PPP-MRSDCI approach, employing both the screened and the standard parameters. All results are in eV units.

| Experiment | Theory (others) | This work |
|------------|-----------------|-----------|
|            | Screened        | Standard  |
| 1.84, 35 1.87, 32, 34 1.91, 39 1.99, 38 3.85, 34 3.86, 35 | 1.65, 46 1.67, 51 1.79, 41 1.83, 43 1.87, 39 1.88, 44 2.18, 35 2.97, 37 3.13, 37 3.25, 37 3.40, 37 | 4.06 (1\(B_{2u}\)) | 4.63 (1\(B_{2u}\)) |
| 3.71, 34 3.78, 37 3.85, 34 3.86, 35 | 6.00, 33 6.33 (1\(B_{2u}\)) | 6.19 (1\(B_{2u}\)) |
| 3.60, 37 | 6.63, 37 | 6.60, 34 6.85 (1\(B_{2u}\)) | 6.73 (1\(B_{3u}\)) |

* DFT(Kohan-Sham) method, ** TDDFT method

RGQD-42

Teranthene is the hydrogen-saturated structural analogue of RGQD-42, for which no experimental, or theoretical data is available, as far as optical absorption spectrum is concerned. However, Konishi et al.\(^ {40}\) have reported the measurement of the absorption spectrum of teranthene with tertiary-butyl group attached on its edge atoms, and the results of their experiments, along with those obtained from our calculations, are summarized in Table IX. In Fig. 6 (a) and (b), we present our calculated spectra of RGQD-42 using the screened, and the standard parameters, respectively, within the PPP-CI approach. If we compare the relative intensity of the first peak of the experimental spectra, we find that results of Konishi et al.\(^ {40}\) are in perfect agreement with our results in that the first peak is not the most intense. However, as is obvious from Table IX, quantitatively speaking, our theoretical results and experimental results of Konishi et al.\(^ {40}\) disagree completely in the low-energy region. Konishi et al.\(^ {40}\) have reported two low-lying excited energy peaks located at 1.17 eV, and 1.21 eV, for which there are no counterparts in our computed spectra. The calculated location of the first peak, which also corresponds to the optical gap, was found to be 1.86 eV from our screened parameter calculation, and 2.04 eV for the standard parameter calculation, as against significantly smaller values 1.17–1.21 eV measured by Konishi et al..\(^ {40}\) As far as higher energy peaks are concerned, Konishi et al.\(^ {40}\) report peaks at 2.96 eV and 3.19 eV, for which again our calculations have no counterparts. The highest measured peak by Konishi et al.\(^ {40}\) is located at 3.87 eV, which is in good agreement both with a screened parameter peak at 3.96 eV, and a standard parameter peak at 3.80 eV. Our calculations predict several peaks in energy region of 4 eV and beyond, which Konishi et al.\(^ {40}\) have not probed. The only possible reason we can think of behind the disagreement between the theory and the experiments in the lower energy region is that the experiments were performed on teranthene saturated with t-butyl group, while our results are valid for hydrogen-saturated material. Nevertheless, we hope that more groups will perform measurements of optical absorption spectra of teranthenes so as to be sure about the value of their optical gap.

Quite expectedly, the many-particle wave function of the 1\(B_{2u}\) state corresponding to the optical gap, obtained from both the standard and the screened parameter calculations, is dominated by the single excitation \(|H \rightarrow L\rangle\). In the spectrum computed using the screened parameters, peak III is most intense, corresponding to a \(B_{3u}\) state located at 3.96, whose wave function is dominated by \(|H - 3 \rightarrow L\rangle - c.c. single excitations. For the standard parameter calculation, peak VII is most intense, corresponding again to a \(B_{3u}\) state, but located at 5.47 eV, with a small mixture of \(B_{2u}\) state located at 5.33 eV. The wave functions of the two states are dominated by single excitations, \(|H - 3 \rightarrow L\rangle - c.c., and \(|H - 1 \rightarrow L + 1\rangle, respectively. The detailed wave analysis of all the excited states contributing
to peaks in the calculated spectra using the screened and the standard parameters, is presented in Tables IX and X, respectively, the Supporting Information.

Table IX: Comparison of calculated peak locations in the optical absorption spectra of RGQD-42, with the experimental results on t-butyl saturated teranthene. No other theoretical results are available for this molecule. Our calculations were performed using the PPP-MRSDCI approach, employing both the screened and the standard parameters. All results are in eV units.

| Experiment | This work |
|------------|-----------|
|            | Screened  | Standard |
| 1.17,1.21, | -         | -        |
| 1.41, 1.57 | 1.86 (1B2u) | 2.04 (1B2u) |
| 2.96       | -         | -        |
| 3.19       | 3.56 (1B2u/1B3u) | -        |
| 3.87       | 3.96 (1B2u) | 3.80 (1B3u) |
| -          | -         | 4.02 (1B2u) |
| -          | 4.15 (1B2u) | 4.21 (1B3u) |
| -          | 4.53 (1B3u) | 4.52 (1B2u) |

RGQD-50

For RGQD-50 and larger structures, it would have been computationally very tedious to perform MRSDCI calculations retaining all the MOs, therefore, we decided to freeze a few lowest-lying occupied orbitals, and delete their electron-hole symmetric highest virtual orbitals. For the case of RGQG-50, we froze/deleted four occupied/virtual orbitals, so that the total number of MOs involved in the calculations reduced to forty-two, same as in case of RGQD-42. In order to demonstrate that this act of freezing and deleting the MOs does not affect the calculated optical absorption spectra, we have performed the calculations for RGQD-50, with four and seven frozen/deleted orbitals, leading to 42/36 active MOs. From the calculated absorption spectra presented in Fig. 7, it is obvious that except for the intensity of the highest energy peak IX in the standard parameter calculations, the spectra remain the same for both the cases, implying that the convergence has been achieved within an acceptable tolerance.

Hydrogen saturated structural analog of RGQD-50 is pentarylene, for which, to the best of our knowledge, no experimental data of optical absorption exists. However, Koch et al.34 have reported the measurements of the absorption spectrum of pentarylene saturated with the t-butyl group, while Baumgarten et al.32 measured only its optical gap. We present our calculated absorption spectra for RGQD-50 in Fig. 6 (a) and (b), while the comparison of important peak locations resulting from our calculations, with the experiments, and other theoretical works is presented in Table X. The value of the optical gap measured by both the groups32,34 is 1.66 eV, which is in very good agreement with the value 1.72 eV computed using the screened parameters, while the corresponding standard parameter value 1.98 eV is on the higher side. If we compare the relative intensity of the first peak of the experimental spectra corresponding to the optical gap, we find that Koch et al.34 report that the first peak to be the most intense one, in disagreement with our results. However, the noteworthy point is that the first peak computed using the screened parameter, is quite intense, and is only somewhat less in intensity than the most intense peak (peak V) of the computed spectrum. As far as higher energy peaks are concerned, Koch et al.34 report peaks at 3.28 eV and 3.45 eV, which are close to a screened parameter peak calculated at 3.39 eV. Next peak reported by Koch et al.34 is at 4.62 eV, which is in good agreement with our standard parameter peak located at 4.71 eV. After that the experimental peak located at 4.80 eV,34 is somewhat close to our screened parameter peak located at 4.97 eV. The next higher measured peak reported by Koch et al.34 is located at 5.29 eV, is in very good agreement with the standard parameter value of 5.34 eV, while screened parameter value of 5.41 eV is slightly larger. Furthermore, we have computed several higher energy peaks as well, for which no experimental results exist. We hope that in future measurements of the absorption spectrum of pentarylene, energy range beyond 5.3 eV will be explored.

On comparing our results to the calculations by other authors, we find that the value of the optical gaps reported by Viruela-Martín et al.46 (1.40 eV) using the valence-effective Hamiltonian approach, Malloci et al.45 (1.54 eV) using the TDDFT method are significantly smaller than our results, as well as experiments. However, Minami et al.44 report a TDDFT value which is in good agreement with the experiment value of the optical gap, but about 0.1 eV lower than our result. Karabunarliev et al.45 computed the optical gap to be 1.97 eV using PM3 semi-empirical method, is in perfect agreement with our standard parameter result located at 1.98 eV, but significantly higher than the experimental value, as well as our screened parameter value. As far as higher energy peaks computed by Malloci et al. are concerned, our PPP model values are in reasonable agreement with them.
The many-particle wave function of the $1B_{2u}$ state corresponding to the optical gap is dominated by the single excitation $|H \rightarrow L\rangle$. In the spectra computed using the screened parameter, peak V is most intense, and is due to a $B_{2u}$ state located at 5.04 eV, along with a small intensity due to a $B_{3u}$ state located at 4.90 eV. The wave functions of the two states are dominated by configurations $|H - 3 \rightarrow L + 3\rangle$, and $|H - 5 \rightarrow L + 1\rangle + c.c.$ excitations, respectively. In the standard parameter spectrum, peak VIII is most intense, and is mainly due to a $B_{2u}$ state located at 6.38 eV, along with a small contribution of a $B_{3u}$ state located at 6.45 eV. The dominant contributions to the many-particle wave functions of these two states are from single excitation $|H - 4 \rightarrow L + 4\rangle$, and the double excitation $|H \rightarrow L + 6; H \rightarrow L + 1\rangle - c.c.$, respectively. The detailed wave function analysis of all the excited states contributing peaks in the spectra computed using the screened and the standard parameters, are presented in Tables XI, and XII, respectively, the Supporting Information.
Table X: Comparison of calculated peak locations in the optical absorption spectra of RGQD-50, with the experimental, and other theoretical results, for pentarylene. The calculations were performed using the PPP-MRSDCI approach, employing both the screened and the standard parameters. All results are in eV units.

| Experiments | Theory (others) | This work |
|-------------|----------------|-----------|
|             |                | Screened  | Standard |
| 1.66, 36, 37 | 1.40, 38, 1.51, 39, 1.54, 40, 1.60, 41, 1.97 | 1.72 ($^1B_{2u}$) | 1.98 ($^1B_{2u}$) |
| 3.28, 34, 3.45 | - | 3.39 ($^1B_{3u}$) | - |
| - | 4.0 | 3.91 ($^1B_{2u}$) | 3.84 ($^1B_{2u}$) |
| - | - | 4.21 ($^1B_{3u}$) | - |
| 4.62 | 4.5 | - | 4.71 ($^1B_{3u}$) |
| 4.80 | 5.2 | 4.97 ($^1B_{2u}$) | 5.12 ($^1B_{2u}$) |
| 5.29 | - | 5.41 ($^1B_{3u}$) | 5.34 ($^1B_{3u}$) |
| - | 6.1 | 5.73 ($^1B_{3u}$) | 5.62 ($^1B_{2u}$) |
| - | - | 5.95 ($^1B_{3u}$) | 5.99 ($^1B_{3u}$) |
| - | 7.4 | - | 6.96 ($^3B_{3u}$) |

For the case of RGQD-54, we performed MRSDCI calculations after freezing/deleting six occupied/virtual MOs, i.e., with forty two active MOs. For this molecule, we were not able to locate any experimental results, or other theoretical calculations, thus, making our results the first ones. We hope that our calculations will give rise to future theoretical and experimental works on this system.

Calculated optical absorption spectra for RGQD-54 are presented in Figs. 6 (a) and (b), obtained using the screened and standard parameters, respectively. The locations of important peaks, and the symmetries of excited states giving rise to them, are summarized in Table XI. The first peak corresponding to the optical gap, is a very weak peak from the theoretical calculations, thus, making our results the first ones. We hope that our calculations will give rise to future theoretical and experimental works on this system.

In the screened parameter calculations, next we find a group of three well-separated peaks, with strong, and almost equal, intensities, located at 2.56 eV, 2.83 eV, and 3.09 eV. The first of these peaks corresponds to an x-polarized transition, while the next two are y-polarized. In the standard parameter spectrum as well, the next three peaks are quite strong, and well separated, but they have their intensities in the ascending order, while the middle peak (peak III) appears as a shoulder of peak IV. The locations of these peaks are blue-shifted compared to their screened parameter counterparts, and are 3.20 eV, 3.69 eV, and 3.98 eV. The polarization characteristics are also different, with two of the peaks exhibiting mixed polarization.

At higher energies, in the screened parameter spectrum there are well defined high-intensity peaks at energies 3.71 eV (x/y polarized), 3.95 eV (x polarized), 5.14 eV (y polarized), and 5.40 eV (x polarized). Out of these the peak located at 5.14 eV (peak IX) is the most intense peak of the computed spectrum. This peak is due to a $B_{2u}$ state, whose wave function is dominated by the singly-excited configuration $|H \rightarrow L\rangle$.

In the standard parameter spectrum, beyond 4 eV, there are a number of low-intensity peaks or shoulders, except for a peak located at 6.56 eV (peak XII), which is the most intense one, and exhibits mixed polarization. This peak is due to a $B_{3u}$ state located at 6.51 eV, along with a smaller contribution to the intensity from a $B_{2u}$ state located at 6.61 eV. The wave functions of the two states are dominated by singly excited configurations, $|H-2 \rightarrow L+7\rangle$+c.c., and $|H-3 \rightarrow L+3\rangle$, respectively.

The detailed wave function analysis of all the excited states contributing peaks in the spectra computed using the standard parameters, and the screened parameters, are presented in Tables XIII, and XIV, respectively, the Supporting Information.
Table XI: The calculated peak locations in the optical absorption spectra of RGQD-54. No other theoretical and experimental results are available for this molecule. Our calculations were performed using the PPP-MRSDCI approach, employing both the screened and the standard parameters. All results are in eV units.

| This work          | Screened          | Standard         |
|--------------------|-------------------|------------------|
| 1.63 (\(1B_{2u}\))| 2.09 (\(1B_{2u}\))|                  |
| 2.56 (\(1B_{2u}\))|                   | -                |
| 2.83 (\(1B_{2u}\))|                   | -                |
| 3.09 (\(1B_{2u}\))| 3.20 (\(1B_{2u}/1B_{3u}\))|                  |
| 3.71 (\(1B_{2u}/1B_{3u}\))| 3.69 (\(1B_{2u}\))|                  |
| 3.95 (\(1B_{3u}\))| 3.98 (\(1B_{2u}/1B_{3u}\))|                  |
| 4.15 (\(1B_{2u}\))| 4.22 (\(1B_{3u}\))|                  |
| 4.31 (\(1B_{2u}\))| 4.60 (\(1B_{3u}\))|                  |
| -                  | 4.97 (\(1B_{3u}\))|                  |
| 5.14 (\(1B_{2u}\))| 5.14 (\(1B_{2u}\))|                  |
| 5.40 (\(1B_{3u}\))| 5.41 (\(1B_{3u}\))|                  |
| 5.60 (\(1B_{3u}\))|                    | -                |
| 5.82 (\(1B_{3u}\))| 5.97 (\(1B_{2u}/1B_{3u}\))|                  |
| -                  | 6.22 (\(1B_{2u}\))|                  |
| -                  | 6.56 (\(1B_{2u}/1B_{3u}\))|                  |

**RGQD-56**

Again, due to a large number of electrons in the system, for RGQG-56 we froze/deleted seven occupied/virtual orbitals, so that the total number of active MOs involved in the calculations reduced to forty-two, same as in case of RGQD-42, RGQD-50, and RGQD-54.

The hydrogen saturated analog of RGQD-56 is quateranthene, for which no experimental measurements of optical absorption spectrum exist. However, Konishi et al. measured the absorption spectrum of quateranthene, with t-butyl groups attached to its edge carbon atoms, with which we will compare our calculated spectra. In Figs. 6 (a) and (b), we present our calculated spectra using the screened and standard parameters, respectively, within the PPP-MRSDCI approach. In Table XII, we present the locations of various peaks in the calculated spectra, and compare them to the measured values of Konishi et al.

If we compare the relative intensity of the first peak of the experimental spectra, we find that the results of Konishi et al. are in perfect agreement with ours in that the first peak is not the most intense. The calculated location of the first peak, which also corresponds to the optical gap, from our calculations was found to be 1.50 eV with the screened parameters, and 1.91 eV with the standard parameters. The experimental value of optical gap reported by Konishi et al. is 1.35 eV, which is about 0.15 eV lower than our screened parameter value, but significantly smaller than the value obtained from the standard parameter calculations. As far as higher energy peaks are concerned, Konishi et al. report several peaks in the range 2.01-2.32 eV, while our calculations do not predict any peaks in that energy region. Next experimental peak located at 3.21 eV, reported by Konishi et al., is in good agreement with our standard parameter peak computed at 3.35 eV. The highest measured peak reported by Konishi et al. is located at 3.46 eV, and it is in reasonably good agreement with a screened parameter peak at 3.61 eV. Furthermore, we have computed several higher energy peaks as well, for which no experimental results exist. We hope that in future measurements of the absorption spectrum of quateranthene, energy range beyond 3.50 eV will be explored.

The many-particle wave function of the \(1B_{2u}\) state corresponding to the optical gap is, as in all previous cases, dominated by the single excitation \(|H \rightarrow L\rangle\). In the spectra computed using screened parameter, peak III is the most intense one, and it is due to a \(B_{2u}\) state located at 2.76 eV, with a smaller contribution to the intensity from a \(B_{3u}\) state located at 2.82 eV. The wave functions of the two states are dominated by doubly-excited configurations \(|H \rightarrow L; H \rightarrow L + 1\rangle\)–c.c., and \(|H \rightarrow L; H \rightarrow L - 2\rangle\)–c.c., respectively. In the standard parameter spectrum, peak V is most intense, and is entirely due to a \(B_{2u}\) state located at 4.34 eV, whose wave function derives most important contribution from the singly-excited configuration \(|H \rightarrow L + 2\rangle\). The detailed wave function analysis of the excited states contributing to various peaks in the spectra computed using the screened and standard parameters is presented in Tables XV, and XVI, respectively, the Supporting Information.
Table XII: Comparison of the calculated peak locations in the optical absorption spectra of RGQD-56, with the experimental results of Konishi et al. No other previous theoretical calculations of absorption spectrum exist for this molecule. The calculations were performed using the PPP-MRSDCI approach, employing both the screened and the standard parameters. All results are in eV units.

| Experiment | This work | Experiment | This work |
|------------|-----------|------------|-----------|
| 1.35, 2.01, 2.10 | 1.50 ($^1B_{2u}$) | 1.91 ($^1B_{2u}$) |
| 2.20, 2.27, 2.32 | - | - |
| - | 2.79 ($^1B_{2u}$/$^1B_{3u}$) | - |
| 3.21 | - | 3.35 ($^1B_{2u}$/$^1B_{3u}$) |
| 3.46 | 3.61 ($^1B_{2u}$/$^1B_{3u}$) | - |
| - | 3.92 ($^1B_{3u}$) | 3.87 ($^1B_{2u}$) |

V. CONCLUSIONS

In this paper, we have presented the results of our very large-scale correlated-electron calculations of spin gaps and optical absorption spectra of rectangular graphene quantum dots, with the number of carbon atoms in the range 28–56, using PPP model Hamiltonian, and the MRSDCI approach. Results of our calculations on the spin gaps of these RGQDs, when extrapolated to infinite graphene, suggest that it has a vanishing spin gap, implying weak electron correlation effects. This result is consistent with the widespread assumption that graphene is a weakly-correlated material.

For the case of optical absorption spectra, we generally found very good agreement with the experiments performed on hydrogen-saturated structural analog of each RGQD, wherever experimental data was available. In certain cases, where no experimental data was available for the H-passivated molecule, the comparison was instead made with the measurements performed on t-butyl group saturated systems, and some quantitative disagreements were encountered, most severe of which were for RGQD-42. It will be very interesting if future experimental measurements could be performed on the H-passivated molecules in those cases. For the case of RGQD-36, and RGQD-54, no experimental measurements exist, while for the case of RGQD-54, even prior theoretical calculations do not exist. Thus, results of our calculations on these molecules could be tested in future measurements of their absorption spectra.

ACKNOWLEDGMENTS

This research was supported in part by Department of Science and Technology, Government of India, under project no. SB/S2/CMP-066/2013.

1. S. Zhou, H. Xu, W. Gan, and Q. Yuan, RSC Adv. 6, 110775 (2016).
2. S.-H. Choi, Journal of Physics D: Applied Physics 50, 103002 (2017).
3. A. Celis, M. N. Nair, A. Taleb-Ibrahimi, E. H. Conrad, C. Berger, W. A. de Heer, and A. Tejeda, Journal of Physics D: Applied Physics 49, 143001 (2016).
4. Y. W. Son, M. L. Cohen, and S. G. Louie, Nature 444, 347 (2006).
5. L. Yang, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. 101, 186401 (2008).
6. V. Barone, O. Hod, and G. E. Scuseria, Nano Letters 6, 2748 (2006), pMID: 17163699, http://dx.doi.org/10.1021/nl0617033.
7. L. Yang, M. L. Cohen, and S. G. Louie, Nano Letters 7, 3112 (2007), pMID: 17824720, http://dx.doi.org/10.1021/nl0716404.
8. J. A. Pople, Trans. Faraday Soc. 49, 1375 (1953).
9. R. Pariser and R. G. Parr, J. Chem. Phys. 21, 767 (1953).
10. A. Shukla, Phys. Rev. B 65, 125204 (2002).
11. A. Shukla, Phys. Rev. B 69, 165218 (2004).
12. P. Sony and A. Shukla, Phys. Rev. B 71, 165204 (2005).
13. P. Sony and A. Shukla, The Journal of Chemical Physics 131, 014302 (2009).
14. H. Chakraborty and A. Shukla, The Journal of Physical Chemistry A 117, 14229 (2013).
15. H. Chakraborty and A. Shukla, The Journal of Chemical Physics 141, 164301 (2014).
16. P. Sony and A. Shukla, Phys. Rev. B 75, 155208 (2007).
17. K. Gundra and A. Shukla, "A pariser–parr–pople model hamiltonian-based approach to the electronic structure and optical
properties of graphene nanostructures,” in Topological Modelling of Nanostructures and Extended Systems, edited by A. R. Ashrafi, F. Cataldo, A. Iranmanesh, and O. Ori (Springer Netherlands, Dordrecht, 2013) pp. 199–227.

18 T. Basak, H. Chakraborty, and A. Shukla, Phys. Rev. B 92, 205404 (2015).
19 T. Basak and A. Shukla, Phys. Rev. B 93, 235432 (2016).
20 K. Aryanzpour, A. Roberts, A. Sandhu, R. Rathore, A. Shukla, and S. Mazumdar, The Journal of Physical Chemistry C 118, 3331 (2014).
21 K. Aryanzpour, A. Shukla, and S. Mazumdar, The Journal of Chemical Physics 140, 104301 (2014).
22 K. Ohno, Theoretica chimica acta 2, 219 (1964).
23 M. Chandross and S. Mazumdar, Phys. Rev. B 55, 1497 (1997).
24 P. Sony and A. Shukla, Computer Physics Communications 181, 821 (2010).
25 R. Buenker and S. Peyerimhoff, Theor. Chim. Acta 35, 33 (1974).
26 R. J. Buenker, S. D. Peyerimhoff, and W. Butscher, Molecular Physics 35, 771 (1978).
27 Y.-W. Son, M. L. Cohen, and S. G. Louie, Physical review letters 97, 216803 (2006).
28 A. Konishi, Y. Hirao, K. Matsumoto, H. Kurata, and T. Kubo, Chemistry Letters 42, 592 (2013), https://doi.org/10.1246/cl.130153.
29 E. Clar and W. Schmidt, Tetrahedron 33, 2093 (1977).
30 S. Arabei and T. Pavich, Journal of Applied Spectroscopy 67, 236 (2000).
31 S. Kummer, F. Kulzer, R. Kettner, T. Baschê, C. Tietz, C. Glowatz, and C. Kryschi, The Journal of Chemical Physics 107, 7673 (1997).
32 M. Baumgarten, K.-H. Koch, and K. Müllen, Journal of the American Chemical Society 116, 7341 (1994).
33 I. Bikhtchantaeva, V. Samartsev, and J. Sepiol, Journal of luminescence 98, 265 (2002).
34 K.-H. Koch and K. Müllen, Chemische Berichte 124, 2091 (1991).
35 R. Ruiterkamp, T. Halasinski, F. Salama, B. Foing, L. Allamandola, W. Schmidt, and P. Ehrenfreund, Astronomy & Astrophysics 390, 1153 (2002).
36 E. Clar and W. Schmidt, Tetrahedron 34, 3219 (1978).
37 T. M. Halasinski, J. L. Weisman, R. Ruiterkamp, T. J. Lee, F. Salama, and M. Head-Gordon, The Journal of Physical Chemistry A 107, 3660 (2003).
38 C. Former, S. Becker, A. C. Grimsdale, and K. Müllen, Macromolecules 35, 1576 (2002).
39 M. S. Gudipati and L. J. Allamandola, life 5, 10 (2006).
40 A. Konishi, Y. Hirao, H. Kurata, T. Kubo, M. Nakano, and K. Kamada, Pure and Applied Chemistry 86, 497 (2014).
41 G. Malloci, ( ), see the UV-Vis absorption spectrum of bisanthene posted at http://www.dsf.unica.it/~gmalloci/pahs/bisanthene/bisanthene.html.
42 M. Parac and S. Grimme, Chemical physics 292, 11 (2003).
43 G. Malloci, G. Cappellini, G. Mulas, and A. Mattoni, Chemical Physics 384, 19 (2011).
44 T. Minami, S. Ito, and M. Nakano, The journal of physical chemistry letters 3, 2719 (2012).
45 S. Karabunarliev, L. Gherghel, K.-H. Koch, and M. Baumgarten, Chemical physics 189, 53 (1994).
46 R. Viruela-Martín, P. M. Viruela-Martín, and E. Orti, The Journal of chemical physics 97, 8470 (1992).
47 G. Malloci, “See the uv-vis absorption spectrum of tetrabenzocoronene posted at http://www.dsf.unica.it/~gmalloci/pahs/tetrabenzocoronene/tetrabenzocoronene.html,” ( ).
Supporting Information for Optoelectronic Properties of Rectangular Graphene Quantum Dots: Pariser-Parr-Pople Model Based Computational Study

Deepak Kumar Rai¹ and Alok Shukla¹,²

¹Department of Physics, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India
²Present Address: Department of Physics, School of Engineering and Applied Sciences, Bennett University, Plot No. 8-11, TechZone II, Greater Noida 201310, Uttar Pradesh, India
In the following tables, we present detailed information about the excitation energies, dominant many-body wavefunctions, and transition dipole matrix elements of excited states with respect to the ground state \((1^1\text{A}_g)\). The coefficient of charge conjugate of a given configuration is abbreviated as 'c.c.' while the sign (+/-) preceding 'c.c.' indicates that the two coefficients have (same/opposite) signs.

Table I. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-28, computed employing the MRSDCI approach, along with the screened parameters in the PPP model Hamiltonian.

| Peak | State | E (eV) | Transition | Dominant Contributing Configurations |
|------|-------|--------|------------|--------------------------------------|
| \(I_g\) | \(1^1\text{B}_2\) | 2.00 | 1.5360 | \(|H \rightarrow L\) (0.8548) \(|H \rightarrow L; H \rightarrow 2 \rightarrow L\)−c.c. (0.0772) |
| \(II_x\) | \(3^1\text{B}_3\) | 3.87 | 1.7616 | \(|H \rightarrow L; H \rightarrow 3 \rightarrow L\)−c.c. (0.5731) \(|H \rightarrow L; H \rightarrow 4 \rightarrow L\)−c.c. (0.1326) |
| \(III_x\) | \(5^1\text{B}_3\) | 4.19 | 1.3240 | \(|H \rightarrow L; H \rightarrow L + 1\)−c.c. (0.4853) \(|H \rightarrow L + 6\)−c.c. (0.1959) |
| \(IV_y\) | \(7^1\text{B}_2\) | 4.49 | 1.5286 | \(|H \rightarrow 2 \rightarrow L; H \rightarrow 2 \rightarrow L; H \rightarrow 1 \rightarrow L + 1\) (0.2613) |
| \(V_x\) | \(11^1\text{B}_3\) | 5.16 | 0.6575 | \(|H \rightarrow 2 \rightarrow L + 1\)−c.c. (0.4371) \(|H \rightarrow L; H \rightarrow L + 1\)−c.c. (0.2663) |
| \(V_{III}\) | \(11^1\text{B}_2\) | 5.28 | 0.2400 | \(|H \rightarrow 4 \rightarrow L + 1\)−c.c. (0.5264) \(|H \rightarrow L; H \rightarrow L + 1\)−c.c. (0.1417) |
| \(VI_x\) | \(15^1\text{B}_3\) | 5.63 | 1.7420 | \(|H \rightarrow 2 \rightarrow L + 4\)−c.c. (0.5536) \(|H \rightarrow L; H \rightarrow 2 \rightarrow L + 3\)−c.c. (0.1496) |
| \(VII_y\) | \(20^1\text{B}_2\) | 6.05 | 1.0110 | \(|H \rightarrow 3 \rightarrow L + 3\) (0.4650) \(|H \rightarrow 4 \rightarrow L + 4\) (0.3576) |
| \(VIII_y\) | \(28^1\text{B}_2\) | 6.41 | 0.7615 | \(|H \rightarrow L; H \rightarrow 5 \rightarrow L + 5\) (0.1877) \(|H \rightarrow 5 \rightarrow L + 5\) (0.5875) |
| \(IX_x\) | \(35^1\text{B}_3\) | 6.83 | 0.3116 | \(|H \rightarrow 3 \rightarrow L + 7\)−c.c. (0.2755) \(|H \rightarrow L; H \rightarrow 10 \rightarrow L\)−c.c. (0.2310) |
| \(X_{x\&y}\) | \(42^1\text{B}_3\) | 7.01 | 0.4071 | \(|H \rightarrow 3 \rightarrow L; H \rightarrow 2 \rightarrow L\)−c.c. (0.2491) \(|H \rightarrow L; H \rightarrow 3 \rightarrow L + 2\)−c.c. (0.2072) |
| \(X_{x\&y}\) | \(41^1\text{B}_2\) | 7.05 | 0.3347 | \(|H \rightarrow 6 \rightarrow L + 3\) + c.c. (0.2771) \(|H \rightarrow L; H \rightarrow 6 \rightarrow L + 1\) + c.c. (0.2136) |
| \(XI_x\) | \(51^1\text{B}_2\) | 7.42 | 0.1846 | \(|H \rightarrow 5 \rightarrow L + 7\)−c.c. (0.2568) \(|H \rightarrow 1 \rightarrow L + 1; H \rightarrow 2 \rightarrow L\)−c.c. (0.1918) |
| \(55^1\text{B}_3\) | 7.45 | 0.3834 | \(|H \rightarrow L; H \rightarrow 7 \rightarrow L + 1\)−c.c. (0.2306) \(|H \rightarrow L + 2; H \rightarrow 1 \rightarrow L + 2\) + c.c. (0.2209) |
Table II. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-28, computed employing the MRSDCI approach, along with the standard parameters in the PPP model Hamiltonian.

| Peak | State | E (eV) | Transition | Dominant Contributing Configurations |
|------|-------|--------|------------|---------------------------------------|
| $I_y$ | $1^1B_{2u}$ | 2.21 | $|H\rightarrow L, H\rightarrow L + 2\rangle + c.c.(0.0849)$ | |
| $II_{x\&y}$ | $4^1B_{2u}$ | 4.06 | $|H\rightarrow L + 5\rangle - c.c.(0.5552)$ | |
| | | | $|H - 1\rightarrow L + 1\rangle (0.2901)$ | |
| | $3^1B_{3u}$ | 4.22 | $|H\rightarrow L + 3\rangle - c.c.(0.4573)$ | |
| | | | $|H \rightarrow L, H - 4\rightarrow L\rangle - c.c.(0.3029)$ | |
| $III_{x\&y}$ | $5^1B_{2u}$ | 4.67 | $|H - 1\rightarrow L + 1\rangle (0.5095)$ | |
| | | | $|H - 2\rightarrow L + 2\rangle (0.3126)$ | |
| | $5^1B_{3u}$ | 4.69 | $|H - 6\rightarrow L\rangle + c.c.(0.3689)$ | |
| | | | $|H \rightarrow L, H - 1\rightarrow L\rangle - c.c.(0.3661)$ | |
| $IV_{x\&y}$ | $8^1B_{3u}$ | 5.06 | $|H\rightarrow L + 6\rangle - c.c.(0.3732)$ | |
| | | | $|H - 2\rightarrow L + 1\rangle - c.c.(0.2678)$ | |
| | $8^1B_{2u}$ | 5.12 | $|H - 1\rightarrow L + 1\rangle (0.4325)$ | |
| | | | $|H \rightarrow L; H\rightarrow L + 2\rangle + c.c.(0.3316)$ | |
| $V_y$ | $10^1B_{2u}$ | 5.41 | $|H - 2\rightarrow L + 2\rangle (0.4009)$ | |
| | | | $|H - 7\rightarrow L\rangle + c.c.(0.3928)$ | |
| $VI_{x\&y}$ | $14^1B_{2u}$ | 5.95 | $|H - 3\rightarrow L + 3\rangle (0.3328)$ | |
| | | | $|H - 4\rightarrow L + 4\rangle (0.2553)$ | |
| | $15^1B_{3u}$ | 6.17 | $|H - 2\rightarrow L + 4\rangle - c.c.(0.5124)$ | |
| | | | $|H \rightarrow L; H - 3\rightarrow L + 2\rangle - c.c.(0.1875)$ | |
| $VII_y$ | $23^1B_{2u}$ | 6.80 | $|H - 5\rightarrow L + 5\rangle (0.5205)$ | |
| | | | $|H - 3\rightarrow L + 3\rangle (0.1825)$ | |
| $VIII_{x\&y}$ | $42^1B_{2u}$ | 7.64 | $|H\rightarrow L; H - 2\rightarrow L + 5\rangle + c.c.(0.2853)$ | |
| | | | $|H - 2\rightarrow L + 8\rangle + c.c.(0.2637)$ | |
| | $44^1B_{3u}$ | 7.69 | $|H - 1\rightarrow L + 1; H\rightarrow L + 4\rangle - c.c.(0.2086)$ | |
| | | | $|H - 3\rightarrow L + 7\rangle - c.c.(0.1962)$ | |
| $IX_x$ | $50^1B_{3u}$ | 7.97 | $|H\rightarrow L; H - 1\rightarrow L + 5\rangle - c.c.(0.2043)$ | |
| | | | $|H - 1\rightarrow L + 1; H\rightarrow L + 4\rangle - c.c.(0.1691)$ | |
| $X_{x\&y}$ | $58^1B_{2u}$ | 8.18 | $|H - 3\rightarrow L + 3\rangle (0.2680)$ | |
| | | | $|H\rightarrow L + 3; H\rightarrow L + 4\rangle + c.c.(0.1792)$ | |
| | $58^1B_{3u}$ | 8.21 | $|H - 6\rightarrow L + 7\rangle + c.c.(0.2280)$ | |
| | | | $|H \rightarrow L + 3; H\rightarrow L + 2\rangle + c.c.(0.1795)$ | |
Table III. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-30, computed employing the MRSDCI approach, along with the screened parameters in the PPP model Hamiltonian.

| Peak | State | E (eV) | Dipole (Å) | Transition Dominant Contributing Configurations |
|------|-------|--------|------------|------------------------------------------------|
| $I_y$ | $1^1B_{2u}$ | 2.11 | 2.3375 | $|H \rightarrow L\rangle \quad (0.8651)$ |
| $II_y$ | $5^1B_{3u}$ | 4.07 | 1.4797 | $|H \rightarrow L; H - 1 \rightarrow L\rangle - c.c. \quad (0.0599)$ |
| $III_y$ | $8^1B_{3u}$ | 4.58 | 0.5733 | $|H \rightarrow L; H - 4 \rightarrow L\rangle + c.c. \quad (0.1246)$ |
| $IV_y$ | $9^1B_{2u}$ | 5.12 | 1.7943 | $|H - 2 \rightarrow L + 2\rangle \quad (0.7819)$ |
| $V_{x}$ | $15^1B_{3u}$ | 5.35 | 1.4599 | $|H - 4 \rightarrow L + 1\rangle - c.c. \quad (0.5163)$ |
| $VI_{x+y}$ | $17^1B_{2u}$ | 5.95 | 0.6331 | $|H - 5 \rightarrow L + 5\rangle \quad (0.5465)$ |
| $VII_y$ | $25^1B_{3u}$ | 6.47 | 0.6478 | $|H - 6 \rightarrow L + 5\rangle \quad (0.3222)$ |
| $VIII_y$ | $33^1B_{3u}$ | 6.86 | 0.3873 | $|H \rightarrow L; H \rightarrow L + 9\rangle + c.c. \quad (0.3376)$ |
| $IX_y$ | $41^1B_{2u}$ | 7.13 | 0.3865 | $|H - 7 \rightarrow L + 7\rangle \quad (0.3649)$ |
| $X_y$ | $47^1B_{2u}$ | 7.35 | 0.2615 | $|H \rightarrow L; H \rightarrow L + 5\rangle + c.c. \quad (0.3426)$ |
Table IV. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-30, computed employing the MRSDCI approach, along with the standard parameters in the PPP model Hamiltonian.

| Peak | State | E (eV) | Dipole (Å) | Transition Dominant Contributing Configurations |
|------|-------|-------|-----------|--------------------------------------------------|
| $I_1$ | $1^1B_{2u}$ | 2.43  | 2.1023    | $|H \rightarrow L\rangle$ (0.8590)               |
|      |       |       |           | $|H - 1 \rightarrow L + 1\rangle$ (0.1237)       |
| $II_{x,y}$ | $3^1B_{2u}$ | 4.64  | 0.3034    | $|H \rightarrow L + 6\rangle$ + c.c. (0.4912)   |
|      |       |       |           | $|H - 1 \rightarrow L + 1\rangle$ (0.3289)       |
|      | $6^1B_{3u}$ | 4.75  | 1.0041    | $|H \rightarrow L + 3\rangle$ - c.c. (0.4511)    |
|      |       |       |           | $|H \rightarrow L; H - 4 \rightarrow L\rangle$ - c.c. (0.2387) |
| $III_x$ | $8^1B_{3u}$ | 5.03  | 0.3272    | $|H \rightarrow L + 7\rangle$ + c.c. (0.4483)    |
|      |       |       |           | $|H \rightarrow L + 5\rangle$ - c.c. (0.2445)     |
| $IV_{x,y}$ | $8^1B_{2u}$ | 5.51  | 0.8169    | $|H \rightarrow L + 2\rangle$ (0.6622)           |
|      |       |       |           | $|H - 1 \rightarrow L + 1\rangle$ (0.2024)       |
|      | $9^1B_{3u}$ | 5.54  | 0.9651    | $|H - 2 \rightarrow L + 1\rangle$ + c.c. (0.5163) |
|      |       |       |           | $|H \rightarrow L; H \rightarrow L + 2\rangle$ + c.c. (0.3113) |
| $V_{x,y}$ | $12^1B_{3u}$ | 5.87  | 0.7562    | $|H \rightarrow L; H \rightarrow L + 4\rangle$ - c.c. (0.3994) |
|      |       |       |           | $|H - 4 \rightarrow L + 1\rangle$ - c.c. (0.2612)  |
|      | $10^1B_{2u}$ | 6.01  | 1.8870    | $|H - 3 \rightarrow L + 3\rangle$ (0.4839)       |
|      |       |       |           | $|H - 4 \rightarrow L + 4\rangle$ (0.3714)       |
| $VI_x$ | $16^1B_{3u}$ | 6.24  | 0.7562    | $|H - 1 \rightarrow L + 4\rangle$ - c.c. (0.4007) |
|      |       |       |           | $|H \rightarrow L; H - 1 \rightarrow L + 5\rangle$ - c.c. (0.2706) |
| $VII_{x,y}$ | $18^1B_{2u}$ | 6.66  | 0.5494    | $|H \rightarrow L; H \rightarrow L + 5\rangle$ (0.5177) |
|      |       |       |           | $|H - 3 \rightarrow L + 3\rangle$ (0.3348)       |
|      | $21^1B_{3u}$ | 6.85  | 1.6773    | $|H - 5 \rightarrow L + 6\rangle$ - c.c. (0.2971) |
|      |       |       |           | $|H - 1 \rightarrow L; H - 5 \rightarrow L\rangle$ - c.c. (0.2522) |
| $VIII_{x,y}$ | $31^1B_{2u}$ | 7.36  | 0.3006    | $|H \rightarrow L; H - 2 \rightarrow L + 5\rangle$ - c.c. (0.2227) |
|      |       |       |           | $|H - 8 \rightarrow L + 1\rangle$ - c.c. (0.2210) |
|      | $28^1B_{3u}$ | 7.40  | 0.5732    | $|H \rightarrow L + 6\rangle$ - c.c. (0.2448)     |
|      |       |       |           | $|H \rightarrow L + 2\rangle$ + c.c. (0.1799)     |
| $IX_{x,y}$ | $36^1B_{3u}$ | 7.77  | 0.4482    | $|H - 7 \rightarrow L + 7\rangle$ (0.3649)       |
|      |       |       |           | $|H - 7 \rightarrow L + 7\rangle$ + c.c. (0.2615)  |
|      | $41^1B_{2u}$ | 7.80  | 0.2955    | $|H \rightarrow L; H - 5 \rightarrow L + 1\rangle$ - c.c. (0.2707) |
|      |       |       |           | $|H \rightarrow L; H - 1 \rightarrow L + 3\rangle$ - c.c. (0.2109) |
Table V. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-36, computed employing the MRSDCI approach, along with the screened parameters in the PPP model.

| Peak | State | E (eV) | Transition | Dominant Contributing Configurations |
|------|-------|--------|------------|--------------------------------------|
| $I_y$ | $1^1B_{2u}$ | 2.11 | $|H \rightarrow L\rangle$ | (0.8489) |
|       |        |       | $|H \rightarrow L + 1\rangle$ | (0.0983) |
| $II_y$ | $3^1B_{3u}$ | 3.63 | $|H \rightarrow L; H \rightarrow L + 1\rangle$ | c.c. (0.5303) |
|       |        |       | $|H \rightarrow L + 6\rangle$ | c.c. (0.1512) |
|       |        |       | $|H \rightarrow L; H \rightarrow L + 1\rangle$ | (0.6509) |
|       | $4^1B_{2u}$ | 3.77 | $|H \rightarrow L; H \rightarrow L; H \rightarrow L + 1\rangle$ | (0.3502) |
| $IV_{x\&y}$ | $5^1B_{2u}$ | 3.96 | $|H \rightarrow L \rangle$ | c.c. (0.5177) |
|       |        |       | $|H \rightarrow L; H \rightarrow L + 1\rangle$ | (0.3355) |
|       | $5^1B_{3u}$ | 4.07 | $|H \rightarrow L; H \rightarrow L + 2\rangle$ | (0.2239) |
| $VI_y$ | $7^1B_{2u}$ | 4.35 | $|H \rightarrow L; H \rightarrow L + 1\rangle$ | c.c. (0.5281) |
|       | $12^1B_{3u}$ | 4.94 | $|H \rightarrow L\rangle$ | c.c. (0.5074) |
|       |        |       | $|H \rightarrow L; H \rightarrow L + 1\rangle$ | c.c. (0.1596) |
| $VII_y$ | $16^1B_{2u}$ | 5.65 | $|H \rightarrow L; H \rightarrow L + 7\rangle$ | c.c. (0.4220) |
|       |        |       | $|H \rightarrow L; H \rightarrow L + 3\rangle$ | (0.3345) |
| $VIII_{x\&y}$ | $24^1B_{3u}$ | 5.99 | $|H \rightarrow L; H \rightarrow L + 5\rangle$ | c.c. (0.4889) |
|       |        |       | $|H \rightarrow L; H \rightarrow L + 3\rangle$ | c.c. (0.2647) |
|       | $21^1B_{2u}$ | 5.99 | $|H \rightarrow L; H \rightarrow L + 1\rangle$ | c.c. (0.6155) |
| $IX_y$ | $28^1B_{2u}$ | 6.50 | $|H \rightarrow L; H \rightarrow L + 5\rangle$ | c.c. (0.3149) |
|       |        |       | $|H \rightarrow L; H \rightarrow L + 3\rangle$ | c.c. (0.6153) |
|       |        |       | $|H \rightarrow L; H \rightarrow L + 1\rangle$ | c.c. (0.4676) |
| $X_x$ | $43^1B_{3u}$ | 6.94 | $|H \rightarrow L; H \rightarrow L + 8\rangle$ | c.c. (0.3827) |
|       |        |       | $|H \rightarrow L; H \rightarrow L + 3\rangle$ | c.c. (0.6155) |
| $XI_y$ | $47^1B_{2u}$ | 7.21 | $|H \rightarrow L; H \rightarrow L + 4\rangle$ | c.c. (0.2177) |
|       |        |       | $|H \rightarrow L; H \rightarrow L + 6\rangle$ | c.c. (0.1931) |
Table VI. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-36, computed employing the MRSDCI approach, along with the standard parameters in the PPP model.

| Peak | State | E (eV) | Dipole (Å) | Transition | Dominant Contributing Configurations |
|------|-------|--------|------------|------------|--------------------------------------|
| Iy   | 1^1B_{2u} | 2.30   | 1.406716   | | |
|      |        |        |            | | |
| II_y| 4^1B_{2u} | 3.87   | 0.913194   | | |
|      |        |        |            | | |
| III_{xy} | 5^1B_{2u} | 4.35   | 0.727174   | | |
|      |        |        |            | | |
| IV_y| 7^1B_{2u} | 4.88   | 1.213884   | | |
|      |        |        |            | | |
| V_y  | 9^1B_{3u} | 5.09   | 1.125146   | | |
|      |        |        |            | | |
| VI_x| 13^1B_{3u} | 5.60  | 0.436946   | | |
|      |        |        |            | | |
| VII_{xy} | 14^1B_{2u} | 5.82  | 0.367347   | | |
|      |        |        |            | | |
|     | 14^1B_{3u} | 5.91   | 1.162591   | | |
|      |        |        |            | | |
| VIII_x| 22^1B_{3u} | 6.57  | 1.624379   | | |
|      |        |        |            | | |
| IX_y| 31^1B_{2u} | 7.00   | 1.129647   | | |
|      |        |        |            | | |
| IX_y| 50^1B_{2u} | 7.78   | 0.466491   | | |
|      |        |        |            | | |
Table VII. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-40, computed employing the MRSDCI approach, along with the screened parameters in the PPP model.

| Peak | State  | E (eV) | Transition | Dominant Contributing Configurations |
|------|--------|--------|------------|--------------------------------------|
| $I_y$ | $1^1B_{2u}$ | 2.02 | 3.1106 | $|H \rightarrow L⟩ +c.c.$ (0.8557) |
| II$_{xk'y'}$ | $4^1B_{2u}$ | 3.97 | 0.7433 | $|H \rightarrow L; H \rightarrow L⟩ −c.c.$ (0.5418) |
| | | | | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.4542) |
| | $6^1B_{3u}$ | 4.16 | 1.4209 | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.5430) |
| III$_{xk'y'}$ | $7^1B_{2u}$ | 4.46 | 0.4448 | $|H \rightarrow L; H \rightarrow L⟩ −c.c.$ (0.4580) |
| | | | | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.4438) |
| IV$_{xk'y'}$ | $10^1B_{2u}$ | 5.16 | 2.0518 | $|H \rightarrow L; H \rightarrow L⟩ −c.c.$ (0.2781) |
| | | | | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.7016) |
| | $16^1B_{3u}$ | 5.17 | 1.1558 | $|H \rightarrow L; H \rightarrow L⟩ −c.c.$ (0.3482) |
| | | | | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.2872) |
| V$_x$ | $25^1B_{3u}$ | 5.88 | 1.3378 | $|H \rightarrow L; H \rightarrow L⟩ −c.c.$ (0.3284) |
| | | | | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.3143) |
| VI$_{xk'y'}$ | $29^1B_{2u}$ | 6.30 | 1.1841 | $|H \rightarrow L; H \rightarrow L⟩ −c.c.$ (0.5752) |
| | | | | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.2588) |
| | $34^1B_{3u}$ | 6.37 | 0.6869 | $|H \rightarrow L; H \rightarrow L⟩ −c.c.$ (0.0682) |
| | | | | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.1899) |
| VII$_{xk'y'}$ | $49^1B_{3u}$ | 6.89 | 0.3030 | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.3611) |
| | | | | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.2973) |
| | $51^1B_{2u}$ | 7.03 | 0.3937 | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.3445) |
| | | | | $|H \rightarrow L; H \rightarrow L⟩ +c.c.$ (0.2926) |
Table VIII. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-40, computed employing the MRSDCI approach, along with the standard parameters in the PPP model.

| Peak | State | E (eV) | Transition | Dominant Contributing Configurations |
|------|-------|--------|------------|--------------------------------------|
| Iy   | $1^1B_{2u}$ | 2.30   | 2.7613     | $|H \rightarrow L\rangle$ (0.8402) |
|      |        |        |            | $|H - 1 \rightarrow L + 1\rangle$ (0.1470) |
| IIy  | $3^1B_{2u}$ | 4.36   | 0.5470     | $|H \rightarrow L + 3\rangle + \text{c.c.}(0.5117)$ |
|      |        |        |            | $|H - 1 \rightarrow L + 1\rangle$ (0.3179) |
| IIIy | $6^1B_{3u}$ | 4.85   | 0.8881     | $|H - 4 \rightarrow L\rangle + \text{c.c.} (0.3945)$ |
|      |        |        |            | $|H \rightarrow L; H \rightarrow L + 5\rangle + \text{c.c.}(0.2458)$ |
| IVxy | $10^1B_{3u}$ | 5.41   | 0.8911     | $|H - 1 \rightarrow L + 2\rangle + \text{c.c.}(0.3678)$ |
|      |        |        |            | $|H \rightarrow L; H \rightarrow L + 2\rangle - \text{c.c.}(0.2935)$ |
|      |        |        |            | $|H - 2 \rightarrow L + 2\rangle (0.6631)$ |
|      |        |        |            | $|H - 8 \rightarrow L + 8\rangle (0.1829)$ |
| Va   | $15^1B_{3u}$ | 5.85   | 0.7202     | $|H \rightarrow L; H \rightarrow L + 5\rangle + \text{c.c.}(0.3695)$ |
|      |        |        |            | $|H - 1 \rightarrow L + 5\rangle - \text{c.c.}(0.2291)$ |
| VIXy | $20^1B_{3u}$ | 6.16   | 0.6527     | $|H \rightarrow L + 1; H \rightarrow L - 2\rangle - \text{c.c.}(0.3325)$ |
|      |        |        |            | $|H - 1 \rightarrow L + 5\rangle - \text{c.c.}(0.2940)$ |
|      |        |        |            | $|H - 4 \rightarrow L + 4\rangle (0.3439)$ |
|      |        |        |            | $|H - 7 \rightarrow L + 7\rangle (0.3086)$ |
| VIIy | $18^1B_{2u}$ | 6.45   | 0.7057     | $|H \rightarrow L; H \rightarrow L + 9\rangle + \text{c.c.}(0.2227)$ |
|      |        |        |            | $|H \rightarrow L + 1; H \rightarrow L + 3\rangle - \text{c.c.}(0.2885)$ |
| VIIIy| $27^1B_{3u}$ | 6.73   | 1.6524     | $|H - 1 \rightarrow L, H \rightarrow L - 2\rangle - \text{c.c.}(0.2650)$ |
|      |        |        |            | $|H - 3 \rightarrow L + 6\rangle + \text{c.c.}(0.2570)$ |
| IXy  | $29^1B_{2u}$ | 7.09   | 0.7071     | $|H - 7 \rightarrow L + 7\rangle (0.2946)$ |
|      |        |        |            | $|H - 14 \rightarrow L\rangle - \text{c.c.}(0.2479)$ |
| XIXy | $42^1B_{3u}$ | 7.56   | 1.4486     | $|H - 7 \rightarrow L + 9\rangle - \text{c.c.}(0.2612)$ |
|      |        |        |            | $|H \rightarrow L + 3; H \rightarrow L + 7\rangle - \text{c.c.}(0.2116)$ |
|      |        |        |            | $|H - 8 \rightarrow L + 8\rangle (0.2639)$ |
|      |        |        |            | $|H \rightarrow L; H \rightarrow L - 12\rangle + \text{c.c.}(0.1783)$ |
| XIx  | $57^1B_{3u}$ | 8.14   | 0.5141     | $|H - 1 \rightarrow L; H - 1 \rightarrow L + 7\rangle - \text{c.c.}(0.1957)$ |
|      |        |        |            | $|H \rightarrow L; H - 3 \rightarrow L + 5\rangle - \text{c.c.}(0.1675)$ |
Table IX. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-42, computed employing the MRSDCI approach, along with the screened parameters in the PPP model.

| Peak | State | E (eV) | Dipole (Å) | Transition Dominant Contributing Configurations |
|------|-------|--------|-----------|-------------------------------------------------|
| $I_y$ | $1^1B_{2u}$ | 1.86 | 2.5210 | $|H \rightarrow L\rangle$ (0.8412) |
| $II_x$ | $1^1B_{3u}$ | 5.30 | 1.2044 | $|H \rightarrow L; H \rightarrow L + 1\rangle$ (0.4984) |
| $IV_y$ | $1^1B_{2u}$ | 3.62 | 1.2714 | $|H \rightarrow L; H \rightarrow L - 2\rangle$ (0.4764) |
| $V_x$ | $1^1B_{3u}$ | 3.96 | 2.1501 | $|H \rightarrow L; H \rightarrow L + 2\rangle$ (0.5100) |
| $VI_y$ | $1^1B_{2u}$ | 4.15 | 2.0730 | $|H \rightarrow L; H \rightarrow L - 1\rangle$ (0.7196) |
| $VII_y$ | $1^1B_{3u}$ | 5.38 | 1.6773 | $|H \rightarrow L; H \rightarrow L - 3\rangle$ (0.5205) |
| $VIII_x$ | $1^1B_{3u}$ | 5.89 | 0.8326 | $|H \rightarrow L; H \rightarrow L - 2\rangle$ (0.1605) |
| $IX_x$ | $1^1B_{2u}$ | 6.25 | 1.2975 | $|H \rightarrow L; H \rightarrow L + 3\rangle$ (0.2374) |
| $39^1B_{3u}$ | 6.34 | 0.9598 | | $|H \rightarrow L; H \rightarrow L - 2\rangle$ (0.2512) |
Table X. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-42, computed employing the MRSDCI approach, along with the standard parameters in the PPP model.

| Peak | State | E (eV) | Dipole (Å) | Transition | Dominant Contributing Configurations |
|------|-------|--------|------------|------------|-------------------------------------|
| I
    | $1^1B_{2u}$ | 2.04 | 2.2700 | $|H \rightarrow L\rangle$ (0.8368) |
| II
    | $4^1B_{3u}$ | 3.80 | 0.4640 | $|H \rightarrow L, H \rightarrow L + 1\rangle$ -c.c.(0.1091) |
| III
   | $5^1B_{2u}$ | 4.02 | 0.8072 | $|H \rightarrow L, H \rightarrow 2 \rightarrow L\rangle$ +c.c.(0.3563) |
| IV
   | $6^1B_{3u}$ | 4.21 | 1.0272 | $|H \rightarrow L + 6\rangle$ +c.c. (0.3059) |
| V
   | $7^1B_{2u}$ | 4.52 | 1.0353 | $|H \rightarrow L; H \rightarrow L + 1\rangle$ (0.4140) |
| VI
   | $9^1B_{2u}$ | 4.76 | 1.6034 | $|H \rightarrow L; H \rightarrow L + 1\rangle$ -c.c.(0.2569) |
| VII
   | $10^1B_{3u}$ | 4.77 | 1.2151 | $|H \rightarrow L; H \rightarrow L - 7 \rightarrow L\rangle$ -c.c.(0.3885) |
| VIII
 | $12^1B_{2u}$ | 5.33 | 0.4950 | $|H \rightarrow L; H \rightarrow L + 1\rangle$ (0.4422) |
| IX
   | $14^1B_{3u}$ | 5.47 | 1.1069 | $|H \rightarrow L; H \rightarrow L - 1 \rightarrow L + 1\rangle$ -c.c.(0.3336) |
| X
   | $19^1B_{3u}$ | 6.03 | 1.0756 | $|H \rightarrow L; H \rightarrow 6 \rightarrow L + 1\rangle$ -c.c.(0.2819) |
| XI
  | $23^1B_{2u}$ | 6.27 | 0.7868 | $|H \rightarrow L; H \rightarrow L - 3 \rightarrow L + 3\rangle$ (0.2978) |
| XII
 | $24^1B_{3u}$ | 6.31 | 1.0124 | $|H \rightarrow L; H \rightarrow L; H \rightarrow 1 \rightarrow L + 2\rangle$ -c.c.(0.2976) |
| XI
  | $29^1B_{2u}$ | 6.52 | 0.5814 | $|H \rightarrow L; H \rightarrow L + 1\rangle$ -c.c.(0.2337) |
| XII
 | $30^1B_{3u}$ | 6.58 | 0.8128 | $|H \rightarrow L; H \rightarrow L - 7 \rightarrow L\rangle$ +c.c.(0.2177) |
| XI
  | $34^1B_{3u}$ | 6.84 | 1.2787 | $|H \rightarrow L + 1; H \rightarrow L \rightarrow 6\rangle$ +c.c.(0.1815) |
| XII
 | $49^1B_{2u}$ | 7.26 | 1.1191 | $|H \rightarrow L; H \rightarrow L + 2\rangle$ -c.c.(0.2013) |
| XI
  | $48^1B_{3u}$ | 7.34 | 1.0043 | $|H \rightarrow L; H \rightarrow L - 8 \rightarrow L\rangle$ (0.3712) |
|      |      |      |            | $|H \rightarrow L + 8\rangle$ (0.3712) |
|      |      |      |            | $|H \rightarrow L + 3\rangle$ (0.2236) |
|      |      |      |            | $|H \rightarrow L \rightarrow L + 6\rangle$ -c.c.(0.2911) |
|      |      |      |            | $|H \rightarrow L + 6\rangle$ +c.c.(0.2512) |
Table XI. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-50, computed employing the MRSDCI approach, along with the screened parameters in the PPP model.

| Peak | State | E (eV) | Dipole (Å) | Transition Dominant Contributing Configurations |
|------|-------|--------|-----------|------------------------------------------------|
| Ig   | 1^1B_{2u} | 1.72   | 3.8432    | [H → L] (0.8590)                                  |
| Hg   | 4^1B_{2u} | 3.39   | 0.9517    | [H → L; H → L + 1] + c.c. (0.0678)                |
| IIx  | 8^1B_{2u} | 3.79   | 0.5483    | [H → L; H → L + 1] + c.c. (0.4451)                |
| III _x & y | 8^1B_{3u} | 4.03   | 1.2328    | [H → L + 4] − c.c. (0.3874)                       |
| IVx  | 11^1B_{3u} | 4.21   | 0.9785    | [H → L; H → L + 3] − c.c. (0.4115)                |
| Vx & y | 20^1B_{3u} | 4.90   | 1.1721    | [H → L; H → L + 3] − c.c. (0.2970)                |
| 17^1B_{2u} | 5.04   | 2.0716  |           | [H → L; H → L + 3] + c.c. (0.2244)                |
| VIx  | 31^1B_{3u} | 5.41   | 1.0791    | [H → L; H → L + 3; H → L + 3] + c.c. (0.1640)    |
| VIIx | 40^1B_{3u} | 5.73   | 0.7423    | [H → L + 1; H → L + 1] − c.c. (0.2227)           |
| VIIx | 50^1B_{3u} | 5.95   | 0.6274    | [H → L; H → L + 1] + c.c. (0.2361)                |
| IXy  | 35^1B_{2u} | 6.23   | 0.8094    | [H → L; H → L + 8] − c.c. (0.2972)                |
Table XII. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-50, computed employing the MRSDCI approach, along with the standard parameters in the PPP model.

| Peak | State \(B_n\) | \(E\) (eV) | Dipole (Å) | Transition Dominant Contributing Configurations |
|------|---------------|-------------|------------|-------------------------------------------------|
| \(I_y\) | \(1^1B_{2u}\) | 1.98 | 3.4780 | \(|H \rightarrow L\) (0.8368) \(|H - 1 \rightarrow L + 1\) (0.1685) |
| \(II_y\) | \(4^1B_{2u}\) | 3.84 | 0.6241 | \(|H - 1 \rightarrow L + 1\) (0.6657) \(|H - 2 \rightarrow L\) + c.c. (0.2916) |
| \(III_x\) | \(8^1B_{3u}\) | 4.71 | 0.8499 | \(|H - 4 \rightarrow L\) + c.c. (0.3818) \(|H \rightarrow L, H \rightarrow L + 5\) - c.c. (0.2012) |
| \(IV_x\) | \(12^1B_{3u}\) | 5.10 | 1.0796 | \(|H - 3 \rightarrow L + 1\) - c.c. (0.3378) \(|H \rightarrow L; H \rightarrow L + 3\) - c.c. (0.2762) |
| \(V_x\) | \(15^1B_{3u}\) | 5.34 | 0.6970 | \(|H - 8 \rightarrow L + 1\) - c.c. (0.3202) \(|H \rightarrow L; H \rightarrow L + 5\) - c.c. (0.2821) |
| \(VI_x\) | \(13^1B_{2u}\) | 5.61 | 1.1140 | \(|H - 3 \rightarrow L + 3\) (0.5543) \(|H - 1 \rightarrow L + 1\) (0.2919) |
| \(VII_x\) | \(18^1B_{3u}\) | 5.64 | 0.7958 | \(|H \rightarrow L; H \rightarrow L + 5\) - c.c. (0.3125) \(|H - 1 \rightarrow L + 5\) - c.c. (0.2359) |
| \(VIII_x\) | \(25^1B_{3u}\) | 5.99 | 0.6481 | \(|H - 1 \rightarrow L + 12\) - c.c. (0.2424) \(|H - 14 \rightarrow L\) + c.c. (0.2348) |
| \(IX_x\) | \(23^1B_{2u}\) | 6.38 | 1.8981 | \(|H \rightarrow L + 4\) (0.3313) \(|H - 9 \rightarrow L + 9\) (0.3307) |
| \(32^1B_{3u}\) | 6.45 | 1.4693 | \(|H \rightarrow L + 6; H \rightarrow L + 1\) - c.c. (0.2247) \(|H \rightarrow L; H - 1 \rightarrow L + 10\) - c.c. (0.1985) |
| \(IX_x\) | \(42^1B_{3u}\) | 6.96 | 0.3205 | \(|H \rightarrow L; H - 2 \rightarrow L + 3\) - c.c. (0.2100) \(|H \rightarrow L; H - 1 \rightarrow L + 4\) - c.c. (0.2050) |
Table XIII. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-54, computed employing the MRSDCI approach, along with the screened parameters in the PPP model.

| Peak | State | E (eV) | Transition | Dominant Contributing Configurations |
|------|-------|--------|------------|--------------------------------------|
| $I_y$ | $1^1B_{2u}$ | 1.63 | 1.4845 | $|H \rightarrow L\rangle \ (0.8330)$ |
|       |        |       |            | $|H - 1 \rightarrow L + 1\rangle \ (0.1286)$ |
| $II_y$ | $2^1B_{3u}$ | 2.56 | 2.2031 | $|H \rightarrow L; H \rightarrow L + 1\rangle +c.c. \ (0.4984)$ |
|       |        |       |            | $|H - 4 \rightarrow L\rangle -c.c. \ (0.1687)$ |
| $III_y$ | $4^1B_{2u}$ | 2.83 | 2.0444 | $|H - 1 \rightarrow L + 1\rangle \ (0.6233)$ |
|       |        |       |            | $|H \rightarrow L; H \rightarrow L; H - 1 \rightarrow L + 1\rangle \ (0.5382)$ |
| $IV_y$ | $5^1B_{2u}$ | 3.09 | 2.1949 | $|H \rightarrow L; H - 2 \rightarrow L\rangle -c.c. \ (0.5340)$ |
|       |        |       |            | $|H - 1 \rightarrow L + 1\rangle \ (0.1943)$ |
| $V_{xy}$ | $9^1B_{3u}$ | 3.66 | 1.9235 | $|H \rightarrow L + 6\rangle +c.c. \ (0.3849)$ |
|       |        |       |            | $|H \rightarrow L; H \rightarrow L + 7\rangle -c.c. \ (0.3397)$ |
| $VI_x$ | $12^1B_{3u}$ | 3.95 | 1.6583 | $|H - 5 \rightarrow L\rangle +c.c. \ (0.5363)$ |
|       |        |       |            | $|H \rightarrow L; H \rightarrow L; H - 1 \rightarrow L + 1\rangle \ (0.1882)$ |
| $VII_y$ | $12^1B_{2u}$ | 4.15 | 0.8667 | $|H - 1 \rightarrow L + 2\rangle +c.c. \ (0.5033)$ |
|       |        |       |            | $|H - 8 \rightarrow L\rangle -c.c. \ (0.1636)$ |
| $VIII_x$ | $17^1B_{3u}$ | 4.31 | 0.7625 | $|H \rightarrow L; H - 2 \rightarrow L + 2\rangle \ (0.4977)$ |
|       |        |       |            | $|H \rightarrow L; H - 7 \rightarrow L\rangle -c.c. \ (0.4137)$ |
|       |        |       |            | $|H \rightarrow L + 6\rangle +c.c. \ (0.2776)$ |
| $IX_y$ | $29^1B_{2u}$ | 5.14 | 1.2230 | $|H \rightarrow L; H - 3 \rightarrow L + 3\rangle \ (0.4616)$ |
|       |        |       |            | $|H \rightarrow L; H \rightarrow L; H - 3 \rightarrow L + 3\rangle \ (0.3651)$ |
| $X_x$ | $39^1B_{3u}$ | 5.40 | 1.4639 | $|H \rightarrow L; H - 2 \rightarrow L + 7\rangle +c.c. \ (0.3768)$ |
|       |        |       |            | $|H \rightarrow L; H - 2 \rightarrow L + 6\rangle -c.c. \ (0.3183)$ |
| $XI_x$ | $43^1B_{3u}$ | 5.60 | 0.6826 | $|H \rightarrow L; H - 2 \rightarrow L + 6\rangle -c.c. \ (0.4033)$ |
|       |        |       |            | $|H \rightarrow L; H - 2 \rightarrow L + 8\rangle -c.c. \ (0.2236)$ |
| $XII_x$ | $48^1B_{3u}$ | 5.82 | 0.6093 | $|H \rightarrow L + 1\rangle -c.c. \ (0.3254)$ |
|       |        |       |            | $|H \rightarrow L + 17\rangle +c.c. \ (0.2814)$ |
Table XIV. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-54, computed employing the MRSDCI approach, along with the standard parameters in the PPP model.

| Peak  | State | E (eV) | Dipole (Å) | Transition | Dominant Contributing Configurations |
|-------|-------|--------|------------|------------|--------------------------------------|
| $I_g$ | $1^1B_{2u}$ | 2.09 | 1.4091 | $|H \rightarrow L\rangle$ | (0.8149) |
|       |       |       |           | $|H \rightarrow L+1\rangle$ | (0.1651) |
|       |       |       |           | $|H \rightarrow L+2\rangle$ | (0.4840) |
|       |       |       |           | $|H \rightarrow L+4\rangle$ | (0.2369) |
| $II_{xy}$ | $2^1B_{3u}$ | 3.15 | 1.6323 | $|H \rightarrow L; H \rightarrow L+1\rangle$ | (0.2515) |
|       |       |       |           | $|H \rightarrow L+1\rangle$ | (0.4851) |
|       |       |       |           | $|H \rightarrow L+2\rangle$ | (0.3073) |
|       |       |       |           | $|H \rightarrow L+3\rangle$ | (0.3495) |
|       |       |       |           | $|H \rightarrow L+4\rangle$ | (0.3201) |
| $III_y$ | $5^1B_{2u}$ | 3.69 | 1.5506 | $|H \rightarrow L+3\rangle$ | (0.4030) |
|       |       |       |           | $|H \rightarrow L+4\rangle$ | (0.3500) |
|       |       |       |           | $|H \rightarrow L; H \rightarrow L+7\rangle$ | (0.3310) |
| $IV_{zxy}$ | $6^1B_{2u}$ | 3.91 | 2.0968 | $|H \rightarrow L+1\rangle$ | (0.3000) |
|       |       |       |           | $|H \rightarrow L+2\rangle$ | (0.2912) |
|       |       |       |           | $|H \rightarrow L+3\rangle$ | (0.4151) |
|       |       |       |           | $|H \rightarrow L+4\rangle$ | (0.3113) |
| $V_x$ | $9^1B_{3u}$ | 4.22 | 1.1430 | $|H \rightarrow L+1\rangle$ | (0.4195) |
|       |       |       |           | $|H \rightarrow L+2\rangle$ | (0.1741) |
| $VI_y$ | $11^1B_{3u}$ | 4.64 | 0.6269 | $|H \rightarrow L+1\rangle$ | (0.3905) |
|       |       |       |           | $|H \rightarrow L+2\rangle$ | (0.2940) |
|       |       |       |           | $|H \rightarrow L+3\rangle$ | (0.2563) |
|       |       |       |           | $|H \rightarrow L+4\rangle$ | (0.2369) |
| $VII_x$ | $14^1B_{3u}$ | 4.97 | 1.0338 | $|H \rightarrow L+1\rangle$ | (0.3414) |
|       |       |       |           | $|H \rightarrow L+2\rangle$ | (0.2686) |
| $VIII_y$ | $14^1B_{2u}$ | 5.14 | 0.9203 | $|H \rightarrow L+1\rangle$ | (0.3850) |
|       |       |       |           | $|H \rightarrow L+2\rangle$ | (0.3640) |
| $IX_x$ | $19^1B_{3u}$ | 5.41 | 0.7882 | $|H \rightarrow L+1\rangle$ | (0.2954) |
|       |       |       |           | $|H \rightarrow L+2\rangle$ | (0.2515) |
| $X_{zxy}$ | $26^1B_{2u}$ | 5.91 | 0.6193 | $|H \rightarrow L; H \rightarrow L+1\rangle$ | (0.2293) |
|       |       |       |           | $|H \rightarrow L+2\rangle$ | (0.2139) |
Table XV. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-56, computed employing the MRSDCI approach, along with the screened parameters in the PPP model.

| Peak | State | E (eV) | Transition Dominant Contributing Configurations |
|------|-------|--------|-------------------------------------------------|
| $I_y$ | $1^1B_{2u}$ | 1.50 | $|H \rightarrow L\rangle$ (0.8452) |
| $H_{15/y}$ | $3^1B_{2u}$ | 2.76 | $|H \rightarrow L; H \rightarrow L + 1\rangle$-c.c. (0.1424) |
| | | | $|H \rightarrow L; H \rightarrow L + 1\rangle$-c.c. (0.5010) |
| | | | $|H - 1 \rightarrow L\rangle$+c.c.(0.2824) |
| $H_{17/y}$ | $2^1B_{3u}$ | 2.82 | $|H \rightarrow L; H - 2 \rightarrow L\rangle$-c.c. (0.5242) |
| | | | $|H - 4 \rightarrow L\rangle$-c.c.(0.2594) |
| $H_{18/y}$ | $8^1B_{2u}$ | 3.61 | $|H \rightarrow L; H \rightarrow L; H - 2 \rightarrow L + 2\rangle$ (0.4553) |
| | | | $|H \rightarrow L; H \rightarrow L; H \rightarrow L + 6\rangle$-c.c.(0.4248) |
| $IV_x$ | $11^1B_{3u}$ | 3.92 | $|H - 1 \rightarrow L + 2\rangle$+c.c. (0.4865) |
| | | | $|H \rightarrow L; H \rightarrow L + 9\rangle$+c.c. (0.1941) |
| $V_{15/y}$ | $11^1B_{2u}$ | 4.32 | $|H \rightarrow L; H \rightarrow L + 10\rangle$-c.c. (0.3907) |
| | | | $|H \rightarrow L; H \rightarrow L; H - 1 \rightarrow L + 1\rangle$ (0.3841) |
| $VI_{15/y}$ | $23^1B_{2u}$ | 4.97 | $|H \rightarrow L; H \rightarrow L + 4\rangle$-c.c. (0.2931) |
| | | | $|H \rightarrow L; H - 4 \rightarrow L + 2\rangle$+c.c. (0.4252) |
| | | | $|H \rightarrow L + 1; H - 2 \rightarrow L + 2\rangle$-c.c. (0.2884) |
| | | | $|H \rightarrow L; H - 1 \rightarrow L + 6\rangle$-c.c. (0.2162) |
| $VII_y$ | $30^1B_{2u}$ | 5.22 | $|H \rightarrow L; H - 2 \rightarrow L + 8\rangle$+c.c. (0.4065) |
| | | | $|H \rightarrow L; H - 4 \rightarrow L + 4\rangle$(0.2276) |
| $VIII_x$ | $49^1B_{3u}$ | 5.88 | $|H \rightarrow L; H - 5 \rightarrow L + 2\rangle$+c.c. (0.4801) |
| | | | $|H \rightarrow L; H \rightarrow L + 1\rangle$+c.c.(0.2123) |
Table XVI. Excited states giving rise to peaks in the singlet linear optical absorption spectrum of RGQD-56, computed employing the MRSDCI approach, along with the standard parameters in the PPP model.

| Peak | State | E (eV) | Transition | Dipole (Å) | Dominant Contributing Configurations |
|------|-------|--------|------------|------------|-------------------------------------|
| $I_y$ | $1^1B_{2u}$ | 1.91 | $|H \rightarrow L⟩$ | 2.8248 | (0.8337) |
| $II_{xy}$ | $3^1B_{2u}$ | 3.32 | $|H \rightarrow L; H \rightarrow L + 1⟩$−c.c. | (0.3783) | (0.1496) |
| | | | $|H − 1 \rightarrow L + 1⟩$ | (0.3586) | |
| | | | $|H \rightarrow L; H − 2 \rightarrow L⟩$+c.c. | (0.4057) | |
| $III_y$ | $5^1B_{2u}$ | 3.87 | $|H \rightarrow L + 7⟩$+c.c. | 1.2282 | (0.4874) |
| | | | $|H − 2 \rightarrow L + 2⟩$ | (0.3066) | |
| | $7^1B_{3u}$ | 4.09 | $|H − 1 \rightarrow L + 1⟩$ | 0.6195 | (0.4561) |
| | | | $|H \rightarrow L + 3⟩$−c.c. | (0.3551) | |
| | $7^1B_{3u}$ | 4.15 | $|H \rightarrow L + 8⟩$−c.c. | 1.3814 | (0.3505) |
| $IV_{xy}$ | $9^1B_{2u}$ | 4.39 | $|H \rightarrow L; H \rightarrow L + 6⟩$−c.c.(0.2916) | 1.7225 | (0.4006) |
| | | $|H − 2 \rightarrow L + 2⟩$ | (0.2769) | |
| | $VI_{xy}$ | $10^1B_{3u}$ | 4.51 | $|H \rightarrow L; H \rightarrow L + 1⟩$−c.c. | 1.0202 | (0.3087) |
| | | | $|H \rightarrow L + 3⟩$−c.c. | (0.2574) | |
| | $11^1B_{3u}$ | 4.63 | $|H \rightarrow L + 2⟩$ | 1.4111 | (0.3934) |
| | | | $|H − 1 \rightarrow L + 1⟩$ | (0.3614) | |
| | $VII_{xy}$ | $15^1B_{3u}$ | 5.09 | $|H \rightarrow L; H \rightarrow L + 1⟩$−c.c. | 0.6254 | (0.3123) |
| | | | $|H \rightarrow L; H \rightarrow 9 \rightarrow L⟩$−c.c. | (0.2352) | |
| | | $|H \rightarrow L; H \rightarrow L + 1⟩$ | (0.4445) | |
| | $13^1B_{2u}$ | 5.20 | $|H \rightarrow L; H \rightarrow L + 1⟩$ | 0.4511 | (0.3259) |
| | | | $|H \rightarrow L; H \rightarrow L + 2⟩$ | (0.2769) | |
| | $VIII_x$ | $17^1B_{3u}$ | 5.38 | $|H \rightarrow L; H \rightarrow L + 1⟩$−c.c. | 0.7487 | (0.3117) |
| | | | $|H \rightarrow L⟩$−c.c. | (0.2132) | |
| | | $|H \rightarrow L; H \rightarrow L + 1⟩$ | (0.3017) | |
| | $IX_{xy}$ | $24^1B_{3u}$ | 5.94 | $|H \rightarrow L; H \rightarrow L + 1⟩$+c.c.(0.3017) | 1.1856 | (0.3091) |
| | | | $|H \rightarrow L + 1⟩; H \rightarrow L − 1 \rightarrow L + 1⟩$ | (0.3329) | |
| | | $|H \rightarrow L; H \rightarrow L + 1⟩$ | (0.2871) | |
| | $24^1B_{2u}$ | 5.99 | $|H \rightarrow L; H \rightarrow L + 1⟩$ | 0.3409 | (0.3017) |
| | | | $|H \rightarrow L; H \rightarrow L + 1⟩$ | (0.3287) | |
| | $X_x$ | $28^1B_{3u}$ | 6.11 | $|H \rightarrow L; H \rightarrow L + 1⟩$ | 0.7549 | (0.3810) |
| | | | $|H \rightarrow L; H \rightarrow L + 1⟩$+c.c. | (0.1974) | |
| | | | $|H \rightarrow L; H \rightarrow L + 1⟩$+c.c. | (0.3264) | |
| | $XI_{xy}$ | $29^1B_{2u}$ | 6.29 | $|H \rightarrow L; H \rightarrow L + 1⟩$+c.c. | 0.4309 | (0.2998) |
| | | | $|H \rightarrow L; H \rightarrow L + 1⟩$+c.c. | (0.2614) | |
| | | | $|H \rightarrow L + 1⟩; H \rightarrow L + 1⟩$+c.c. | (0.3028) | |
| | $34^1B_{3u}$ | 6.39 | $|H \rightarrow L; H \rightarrow L + 1⟩$ | 1.2890 | (0.2642) |
| | | | $|H \rightarrow L; H \rightarrow L + 1⟩$+c.c. | (0.2555) | |
| | | | $|H \rightarrow L; H \rightarrow L + 1⟩$+c.c. | (0.2050) | |
| | $XII_{xy}$ | $41^1B_{3u}$ | 6.67 | $|H \rightarrow L; H \rightarrow L + 1⟩$+c.c. | 0.7789 | (0.3114) |
| | | | $|H \rightarrow L; H \rightarrow L + 1⟩$+c.c. | (0.2800) | |
| | | | $|H \rightarrow L; H \rightarrow L + 4⟩$ | (0.3114) | |