



Mach-Zehnder quantum interference rules in hydrocarbons with substituents

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Abstract

We have investigated the conditions of quantum interferences in hydrocarbons with substituents using density functional theory and tight binding approximation combined with non-equilibrium Green's function technique. The chosen model systems, namely benzene and tripyridyl-triazine molecules, have elucidated three prominent rules. The '*first rule*' is the occurrence of inevitable, destructive quantum interference when 1,3-benzene ring incorporates single substituent at the fifth site. The '*second rule*' is the chaotic occurrence of quantum interferences due the position and/or type of the substituents. The '*third rule*': the substituents decrease (increase) the probability of destructive (constructive) interferences

Keywords

Mach-Zehnder, Quantum interference rules, Hydrocarbons, Substituents

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1. Introduction

Exploiting quantum interference (QI) in molecular electronics represents a pivotal factor that essentially defines the quality of future electronic circuits [1–4]. These metal-molecule-metal devices allow electrons to pass from one electrode to the other via a central molecule in a coherent phase [5–9]. As a result, quantum interferences occur between wavefunctions of the passing electrons and wavefunctions of the molecule localized states. These interferences appear in the spectra of the transmission probability as specific patterns, such as Fano [10–14], Breit-Wigner [15–17], and Mach-Zehnder [18,19] resonances. The electronic resonances can substantially be controlled [11,20,21] utilizing advanced fabricating schemes such as chemical modification [22] so that the consequent electrical conductance of nanoscale devices can be effectively ameliorated [23–25]. Therefore, understanding QI and the corresponding controlling conditions formulate the limits for practical engineering of advanced molecular junctions. A well-known strategy used to tune the electrical properties of molecular junctions is to adjust the resonances of the transmission in the vicinity of the Fermi level [23,26]. A typical approach to employ such a strategy is Mach-Zehnder quantum interactions. These interferences emerge from the recombination of sub-waves resulting from a single incoming de Broglie wave when it enters a multipath junction. The shattered fractions of the original incident wave suffer from phase shifting because they have flown through different paths with different lengths before they completely merge again [18]. For instance, cyclic-molecules such as benzene exhibit variations in their conductance (σ) values as a consequence of para, meta, and ortho ($\sigma_{para} > \sigma_{ortho} > \sigma_{meta}$) connections [18,27–31]. Thus, the ability to manipulate Mach-Zehnder QI represents a promising technique to control the electrical properties of nano-junctions. Researchers worldwide have previously focused on the general rules of Mach-Zehnder resonances and their tuning conditions in, for example, electronic [32–38] and optoelectronic circuits [39–41]. On the other hand, Garner et al. [42] have found that QI patterns do not follow the traditional para, meta, and ortho rules of hydrocarbons when a single substituent is introduced in the parent molecule. Furthermore, Sangtarash et al. reported similar unusual behavior when a nitrogen atom is deliberately substituted in the structure of

polyaromatic hydrocarbons [43]. Hence, this work aims at mapping the new QI behavior in hydrocarbons with substituents. To fulfill such aim, we have investigated QI patterns in a benzene ring and a recently fabricated tripyridyl–triazine (TPTZ) molecule [44]. In the case of the benzene molecule, we investigated 25-doped configurations and three classical intact para-, meta-, ortho-connected structures. The present results denote three rules in the currently studied molecules. Rule-1, introducing one heteroatom may increase the conductance by two orders. Rule-2, the type and location of the substituent generate unpredictable manifestation of QI. Rule-3, inevitable and invariant DQI associates with the substituent location—site 5 in benzene—regardless of the connectivity type (para, meta, or ortho). We have also found that the probability of destructive QI descends significantly from 35% in pure benzene to less than 10% in doped rings. Therefore, the rules envisage QI and electrical conductance in hetero-hydrocarbons provided that the type and location of the hetero-atom and the connectivity of the backbone molecule are predefined.

2. Theoretical methods

The density functional theory within the quantum chemistry package (SIESTA) [45] has been employed to optimize the structure of benzene and tripyridyl–triazine molecules. We have added thiol (SH) moiety as a linker in the case of benzene alone. Thus, in the case of benzene, the term “molecule” will refer to the benzene-dithiol unit. The optimization uses the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional for exchange and correlation [46], double zeta polarized (DZP) basis sets for the atoms of the molecule plus anchor (carbon, nitrogen, hydrogen, and sulphur), and double zeta (DZ) basis sets for the gold atoms of the leads. Such a reduction in the size of the basis sets of the leads' atoms saves time and insignificantly affects the conductance [47]. In addition, the DFT calculations implemented norm-conserving pseudopotentials and real space grid with 200 Rydberg mesh cut-off. Each molecule, benzene-dithiol or TPAZ, was first optimized in the gas phase and considered fully relaxed when all forces on atoms were below 0.04 eV/Å. The leads consist of 84 Au atoms and extra four Au atoms added to each surface close to the molecule. The role of these four extra Au adatoms at the surfaces is to

create an Au tip directly facing the molecule to eliminate any dependence of the transmission on the structure of the contacts [48]. The adopted Au-adatoms structure does not mean that our results will be different for flat or irregular leads, it only means that the present calculations were done under the most highly reduced variations. Then, the optimum bond length between the tips' atoms of the leads and the molecule was obtained by varying the distance between them until the whole system reaches its minimum energy. The thiol units interact directly with the gold leads due to their strong Au–S bonds (2.4 Å) [49] after losing their hydrogen atoms [50,51]. At the optimized distance, we attached the molecule to the Au adatoms, kept the system frozen, and ran SIESTA to yield a mean-field Hamiltonian of the system. The Hamiltonian was then used to calculate the electrical properties of the molecule using GOLLUM, a quantum transport code based on the non-equilibrium Green function (NEGF) method [52].

In the phase-coherent condition, GOLLUM calculates the transmission coefficient $T(E)$ of the molecular junction using the relation, $T(E) = \text{Tr}[\Gamma_R(E)G^R(E)\Gamma_L(E)G^{R\dagger}(E)]$, where, $\Gamma_{R,L}$ is the level broadening which arises from the interaction between the molecule and both right (R) and left (L) leads. The retarded Green function is $G^R = (ES - H_s - \sum L - \sum R)^{-1}$, where E is the energy, H_s is the Hamiltonian of the scattering region, S is the overlap matrix, and $\sum_{L,R}$ is the self-energy of the left (right) lead. Using Landauer formula, the electrical conductance takes the form, $\sigma(E) = \sigma_o \int T(E)[-\partial_E f(E)]dE$, where $\sigma_o = 2e^2/h$ is the quantum conductance, $f(E)$ is the Fermi-Dirac function, e is the electron charge, and h is Planck's constant [52].

To have insight into the DFT outputs, we calculated the transmission coefficient of tight-binding (TB) models of benzene and TPTZ molecules. These calculations are reasonably accurate, inexpensive, and straightforward since the models are defined by allocating onsite energy for each site, considering coupling energy with all first neighbor sites, and neglecting all coupling elements between any non-adjusted sites. GOLLUM can perform first-order TB calculations, however, we preferred using Olife code. It requires simple inputs, offers a friendly Graphical User Interface (GUI), and takes efficiently short time to produce transmission data. Furthermore, Olife similarly follows the same Green function approach that is incorporated in GOLLUM. More detail about Olife and its methodology can be found in Ref. [53].

3. Results and discussion

To present a systematic study of the effect of substituents on molecular QI, we have considered the most possible locations of the dopants in the structure of the benzene ring. All structures with and without substituents were 28 models, see Fig. 1. We took advantage of the symmetry of the molecule so that repeated structures were omitted. For example, the substituted site in model 4 (M4), Fig. 1, may take the locations two, three, five, and six. However, due to symmetry, we have only considered position two. Fig. 1 also shows that the first three cases refer to the previously mentioned para-, meta-, and ortho-connections, respectively, while the other 25 structures represent other probable sites that the substituents may occupy. For simplicity, the substituted site of the benzene was represented by a single heteroatom (nitrogen); however, these substituents may take different chemical formulae, and/or multiple dopants may simultaneously take various locations [42]. Within the formula of the tight-binding (Hückel) model, the substituent is simulated by allocating onsite energy to the specified site different from the rest of the other sites. For instance, the substituent (nitrogen atom) in Fig. 1 was set to be equal to 1.00 while all other onsite energies were zeros. The coupling matrix elements in the 28 models were -1.00 in both left and right leads, -0.50 in the molecule's rings, -0.40 between rings, and -0.30 between the left/right lead and molecule. It is worth mentioning that the above onsite and coupling energies were fixed for all structures and the only variables we had changed were the number of substituents and their potential locations.

Comparing the transmission coefficients at the center of the band of panels (a) and (c) in Fig. 2 illustrates convergent values near the predicted Fermi energy. Such a trend is inconsistent with previous theoretical calculations of Bauschlicher et al. [47] and Sangtarash et al. [54]. The former studied the effect of chlorine substituents on the current–voltage curve of 1,4-benzedithiol molecule, and the latter elicited the impact of nitrogen on thermoelectric properties of hydrocarbons. Besides, we have obtained a reasonable agreement with the experimental results of Venkataraman et al. [55]. However, Venkataraman et al. showed different arrangements of CH_3 substituent, where they have found that the conductance increases with the number of substituents. In other words, the conductance (σ) of 1,4-diaminobanzen would have the following sequence: $\sigma_{(4 \times \text{CH}_3)} > \sigma_{(2 \times \text{CH}_3)} > \sigma_{(1 \times \text{CH}_3)}$ [55]. In comparison, we find that

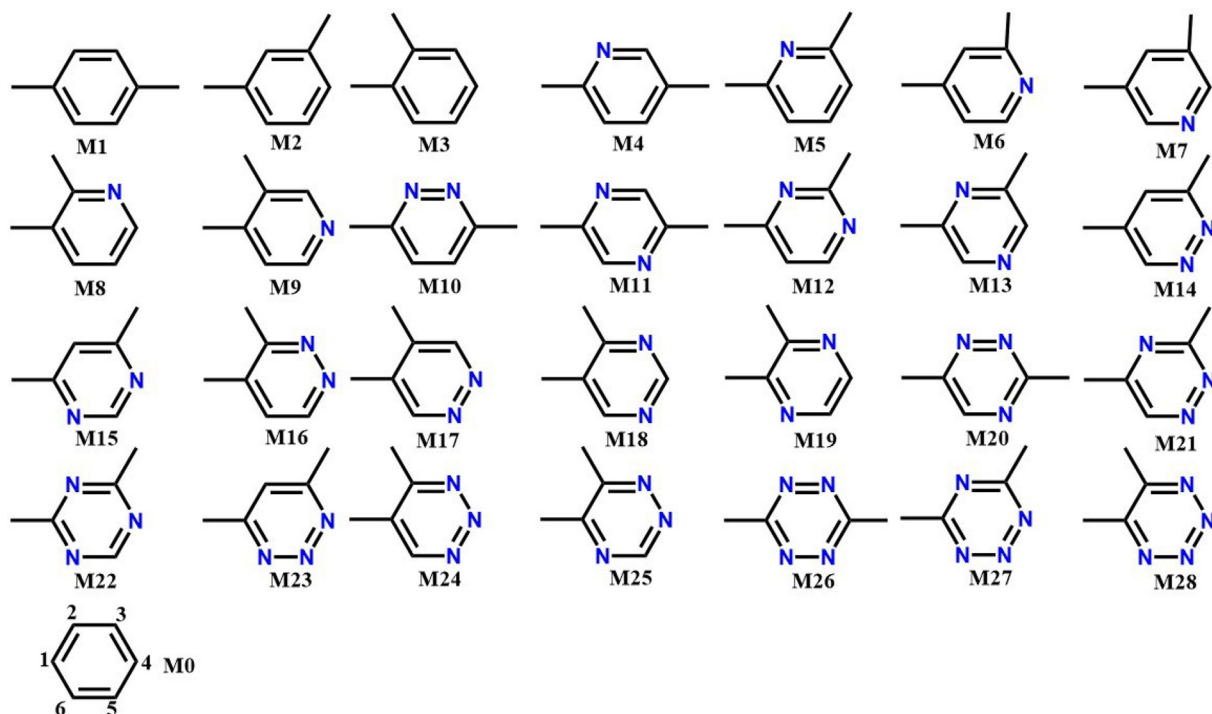


Fig. 1. Illustrates the most possible locations for the substituent (nitrogen atom) to embed in the benzene molecular structure. The last model (M0) depicts the labeling of the benzene, such that all other structures similarly follow.

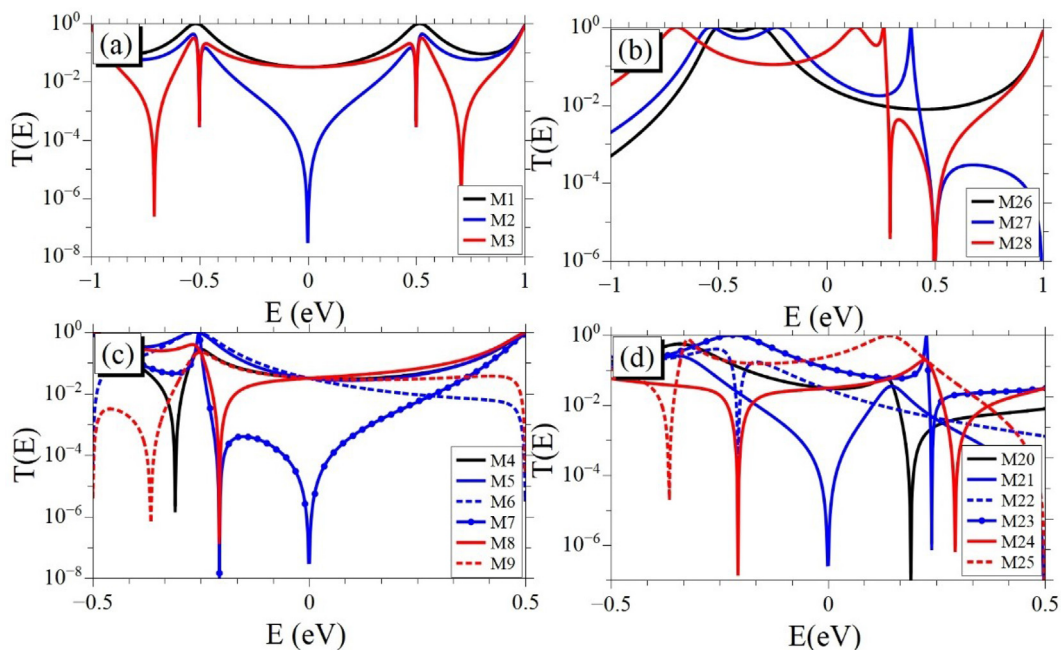


Fig. 2. Tight binding transmission coefficient corresponds to benzene models shown in Fig. 1. In all panels, the black, blue, and red curves represent models with para-, meta-, and ortho-connection, respectively.

$\sigma_{(2 \times CH_3)} > \sigma_{(1 \times CH_3)} > \sigma_{(4 \times CH_3)}$, which is similar to the same measurements of 2-fluoro-1,4-diaminobenzene and 4-fluoro-1,4-diaminobenzene [55]. Furthermore, we obtained a reasonable agreement with the experimental measurements of Vazquez et al. but not with the theoretical results [56]. The group of Vazquez measured the conductance of was 1,4-bis(methyl (thio) methyl)–benzene. They connected the main benzene ring to external electrodes in para-connection, and they separately studied the effect of adding four fluorine (F) atoms and single methoxy (OMe) unit on the conductance of the junction. Experimentally, Vazquez et al. found that the conductance take the following consequence: $\sigma_{pure} = \sigma_{OMe} > \sigma_{(4 \times F)}$ whereas, the theory calculations presented different sequence, $\sigma_{(4 \times F)} > \sigma_{pure} > \sigma_{OMe}$, see table (1) in Ref. [56]. Such controversial results of the transmission imply a very complicated phenomenon governed by a large number of variables including: the position, type and conformation of the substituent and molecule, the surrounding environment, together with the formation and quality of the connection between the active molecule and the leads. Therefore, one cannot always simply deduce the behavior of the transmission coefficient of doped hydrocarbons.

The second model system is tripyridyl–triazine, TPTZ. The reason for choosing the TPTZ molecule is firstly related to the engineering of conventional electronic units, such as amplifiers [57] and transistors, which require a three-terminal component. Therefore, we have chosen a molecule with three-link groups that can be attached to three external electrodes, namely source, drain, and gate [58–61]. The second reason is the general analogy between the TPTZ core unit, so-called triazine, and benzene ring. In other words, the structure of TPTZ can be decimated to look like model M27 of the benzene ring in which two carbons were attached to two external leads, and the left four carbon atoms were substituted/doped, see Fig. 1. Similarly, using the DFT and TB, we have investigated the electrical characteristics of TPTZ as shown in Fig. 3. Experimental measurements of the electrical conductance of TPTZ done by Iwane et al. reveal three distinctive conductance states (high, medium, and low) depending on the path length which the current takes through the molecule [44]. A high conductance state (shortest path) emerges when the input lead and output lead are attached to the central triazine unit. Triazine ($C_3H_3N_3$) is similar to the benzene ring but contains three nitrogen atoms and three carbon atoms attached to three correspondent hydrogen atoms.

The medium state (the modest path) occurs when one of the leads is attached to the central ring, and the other lead is connected to one of the external rings. The low conductance state (the longest path) results from the configuration in which both leads were linked to different peripheral rings. A very prominent feature of all configurations of the TPTZ is the pinned peak close to the Fermi level of the leads. The literature clearly shows that this feature is generic in the molecules containing nitrogen [50]. To verify the effect of nitrogen atoms on the transmission, we have first considered a model system without any dopant. Such a pure hydrocarbon molecule named 1,3,5-triphenylbenzene (TPB) is similar to the TPTZ molecule but without any nitrogen atoms. Fig. 3c shows the transmission of the TPB molecule, which presents symmetric transmission curves with two destructive QI at the Fermi level due to the meta connection. However, when we changed the onsite energy of the model system to simulate the TPTZ molecule, we can see a fixed peak next to the Fermi level appears prominently, as shown in Fig. 3b. Therefore, we deduce that the resonance next to the Fermi level is primarily related to the dopant and minorly to the geometry of the molecule.

The next characteristic of Fig. 3 is that all destructive QI disappears as a result of the incorporation of the substituents in the molecular structure of TPTZ. This disappearance can be viewed in terms of the structure of similar models such as M27 and M28, which clearly do not show any destructive interference, see Fig. 2. Furthermore, the conductance of M27 is less than the conductance of M28, a behavior that echoes the low and medium states of TPTZ, respectively.

4. Conclusions

Using density functional theory and nearest neighbor tight bind method, we have investigated quantum interference rules in 30 molecules, including benzene, tripyridyl–triazine, and 1,3,5-triphenylbenzene. We have found that for the chosen tight binding conditions, destructive quantum interferences only appear in two (meta attached) 1,3-six-numbered models. The benzene model shows destructive QI when a single substituent occupies site number five, and the tripyridyl–triazine model exhibits destructive QI when it incorporates three substituents at sites two, four, and five. Besides, the results show (*Rule-3*) that adding substituents to hydrocarbons decreases the probability of occurrence of destructive quantum interferences to less than 10% in benzene molecule and zero percent in tripyridyl–triazine molecule. *Rule-2*

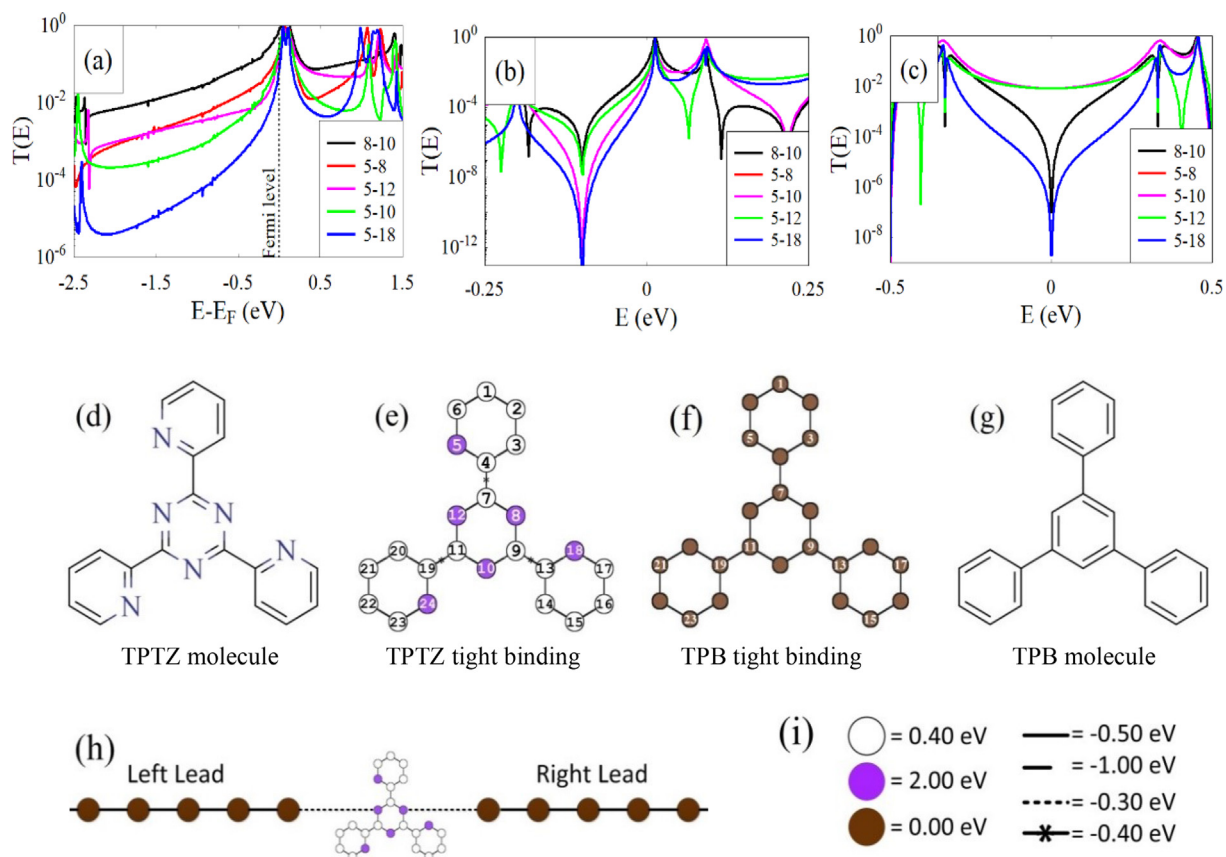


Fig. 3. (a) DFT-calculated transmission coefficient of (d) TPTZ molecule. (b) and (c) TB-calculated transmission coefficient of (e) TPTZ and (f) TPB tight binding models, respectively. Panel (g) shows molecular structure of TPB. Panel (h) is the TB representation of the junction (left lead-molecule-right lead). The values of the TB parameters used in (b, c, e and f) are listed panel (i).

points out to the unpredictable behavior of quantum interferences due to the position and type of substituents. The last rule (*Rule-1*) is the appearance of a single, invariant, destructive QI associated with a site-five-substituted 1,3-benzene molecule. The present results reveal that doping the functional molecule with one heteroatom can generally enhance the conductivity by approximately two orders. The study also determines the locations we should care about to avoid or create destructive QI and to tune the electrical conductance.

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