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Can Molecular Quantum Interference Effect Transistors Survive Vibration?

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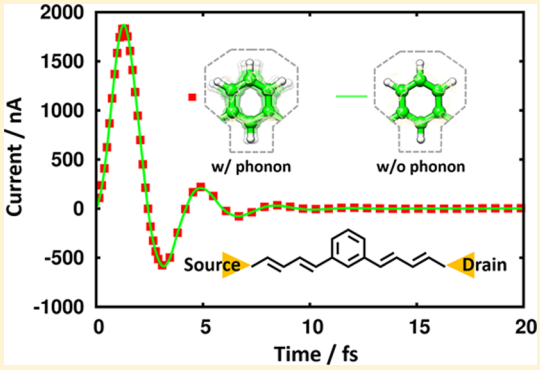
Supporting Information

ABSTRACT: Quantum interference in cross-conjugated molecules can be utilized to construct molecular quantum interference effect transistors. However, whether its application can be achieved depends on the survivability of the quantum interference under real conditions such as nuclear vibration. We use two simulation methods to investigate the effects of nuclear vibration on quantum interference in a meta-linked benzene system. The simulation results suggest that the quantum interference is robust against nuclear vibration not only in the steady state but also in its transient dynamics, and thus the molecular quantum interference effect transistors can be realized.



As the size of metal oxide semiconductor field effect transistors (MOSFET) inches toward the physical limits, the emerging quantum effect causes trouble in the circuits design with traditional silicon-based semiconductors. To overcome this challenge, scientists brought up the idea of using single molecules[1,2] as electronic devices and have made great efforts in both experimental and theoretical research. The breakthroughs in scanning tunneling microscopy (STM) and atomic force microscopy (AFM) facilitate relevant research activities and provide insight into the transport properties of the molecular devices when combined with mechanically controllable break junction (MCBJ) techniques.[3,4] In theoretical studies, the success in nonequilibrium Green's Function (NEGF) techniques and density functional theory (DFT) offers scientist powerful tools for simulating charge transport through molecular junctions.[5] Molecular electronic devices with unique functions or operating mechanisms are also explored widely,[6−9] among which certain types of molecular structures have attracted considerable attention from many research groups.[10−18] In these structures, multiple charge-transport pathways are created by utilizing π-conjugated rings in molecular junctions. When the pathways are equal, interference manifests itself in a constructive way and facilitates charge transport, for example, para-linked benzene. If the phase difference between the pathways is equal to π, then destructive interference occurs, which forbids the electrons from passing through, as exemplified by meta-linked benzene or other cross-conjugated molecules. The low transmissions caused by phase cancellation near the Fermi level are well understood.[19] Time-dependent simulations suggest that it requires time for the electrons from the two paths to reach the electrode where measurement takes place and the role of quantum interference (QI) is observed.[20] For more complicated molecules, a simple graphical scheme is proposed to predict the existence of QI-induced transmission cancellation.[10] Theoretical studies on the conductance of benzene-based molecular devices and extended structures suggest that QI can be utilized to construct molecular quantum interference effect transistor (QuIET), in which the conductance of the molecular device is modulated by introducing decoherence or elastic scattering.[21] Other researchers tried to control anthraquinone-based molecular switches through electrochemical reaction or electric field.[22−24] Although molecular electronics have great potentials, several problems have to be tackled before practical application, such as mass production of single molecular devices, reproducibility of the electrical contacts, and the conductance measurements.[25,26] Great efforts made to solve these problems have resulted in much progress.[27−29] However, one issue has not been addressed very clearly, namely, the influence from nuclear vibration on electronics. In the presence of phonons, the dephasing caused by inelastic scattering may intervene with the coherent electron transport process and reduce the effectiveness of the QuIET. Although the influence of the electron−phonon interactions (EPIs) on quantum electron transport has been evaluated in previous works,[30−32] few were concerned about the robustness of QI in molecular junctions against

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nuclear vibration.[33,34] The effect of EPI on QI is yet to be clarified.

To answer this question in this manuscript, Ehrenfest molecular dynamics (EhMD)[35] is carried out on a benzene molecule with electrodes attached to meta-positions, and the vibrational effect on the current is examined. The simulation results are compared and confirmed by another method in which the nuclear vibrations are accounted for by introducing a self-energy in NEGF formalism.[36−40] Among the two methods, the Ehrenfest molecular dynamics describes the nuclear motions explicitly and therefore is more intuitive. The self-energy treatment of the electron−phonon interaction, on the contrary, has the advantage of solving both the electrons and the nuclei quantum mechanically and therefore is expected to be more accurate. Details of the two methods can be found in the Supporting Information.

Figure 1 shows the schematic diagram of the system being investigated. A benzene molecule is attached to two electrodes

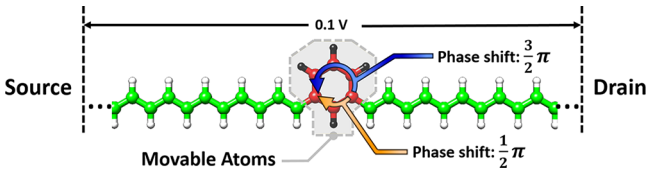

Figure 1. System being investigated is a benzene molecule attached to two semi-infinite extended alkene chains through meta-positions. When the nuclei are fixed, the phase difference between the two paths equals π. The resulting destructive interference prevents the electrons from passing through the molecular junction. In simulations for examining the effect of nuclear vibration, 10 atoms in the benzene ring colored in red or black are set to be movable. The bias voltage across the device region is 0.1 V.

made of semi-infinite extended alkene chain of equal bond length through meta-positions. The electrode is chosen so that the influence of σ tunneling that weakens the destructive interference can be excluded.[41] 10 atoms in the benzene ring colored in red or black are set to be movable, which is a reasonable simplification because it covers the two complete paths needed for the destructive QI. To obtain a reliable result, 260 EhMD calculations are carried out independently with initial velocities set randomly following the Maxwell distribution at 300 K. Bias voltage is applied exponentially with respect to time with an amplitude of 0.1 V, that is, $V(t) = 0.1\ \mathrm{V}(1 - \mathrm{e}^{-t/a})$, where the time constant a is set to 0.5 fs. Wide-band limit approximation is adopted to account for the self-energies due to the electrodes.

In all 260 EhMD trajectories, an overshoot of the current can be observed in the first few femtoseconds. After that, the current fluctuates around a certain value due to the nuclear motion. The red solid line in Figure 2a shows the time-dependent current in a typical EhMD trajectory. The maximum amplitude of the oscillations after the overshoot is ∼140 nA, which is a fairly large value compared with the steady-state current without nuclear motion (∼1.2 nA). Picking the coordinates of the nuclei frame by frame from the above-mentioned EhMD trajectory and fixing them for steady-state calculations, we obtain the currents in the adiabatic limit. The results are plotted as the blue dotted line in Figure 2a, with its magnification shown in the inset. It is found that the steady-state currents are always quite small (<3.5 nA), revealing the robustness of the QI against static distortions. The results can

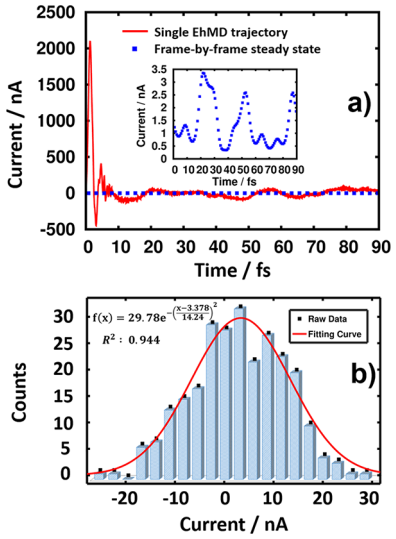

Figure 2. EhMD simulation results of the meta-linked benzene system. (a) The red line is the time-dependent current obtained from a typical EhMD trajectory; the blue dotted line represents the current from frame-by-frame steady-state calculations with fixed nuclei whose coordinates are picked from the trajectory mentioned above. The inset figure shows the same blue dotted line magnified. (b) For each of the 260 EhMD current trajectories, the average is taken over the time period of 20−90 fs. After that, the 260 average values of the current are binned into 20 sections to generate a histogram that approximates a normal distribution.

be understood by a simple Hückel model in which the hopping values are approximately proportional to the overlaps of adjacent orbitals. When bonds in the benzene ring are distorted or broken, in many cases, new cross-conjugated structures are created and the electron transport is still inhibited. In other cases, it is not until the hoppings are tuned to below 1/10 of their original values that the destructive QI is effectively suppressed. Such extent of distortions is almost impossible in realistic situations. Therefore, the large deviation between the EhMD and the frame-by-frame steady-state results can only be attributed to the time-dependent effects of the nuclear motions rather than the static geometric changes.

To evaluate the influence of the nuclear vibration on steady-state current, we now focus on the time period after the overshoot. In the reference system with nuclei being fixed at the optimized configuration, the average of the current was taken over the time period of 20−90 fs and gives a result of 1.0 nA. The same procedure was repeated for each of the 260 EhMD current trajectories. The 260 average currents have a mean value of 1.6 nA, which, when compared with the steady-state current of the fixed nuclei dynamics, has only a small difference. This difference was further confirmed to be insignificant by a statistical analysis. First, a bootstrap method was employed to investigate the reliability of the mean value. An ensemble of 100 000 Monte Carlo resampling gives an estimated standard error of 0.59 nA, which agrees well with the 0.6 nA difference. A closer look at the 260 average currents reveals further trends. In Figure 2b, the raw data were binned into 20 sections to generate a histogram that approximates a normal distribution with a coefficient of determination (R^2) of 0.944. The standard error under the normal distribution assumption is 0.59 nA. Therefore, the conclusion can be made that the destructive QI in meta-linked benzene system is robust against the nuclear vibration.

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To verify our findings, we carry out simulations on the same structure but with a different method to account for the nuclear vibration, that is, quantum mechanically describe the influence of nuclear vibration on electrons by introducing the self-energy due to EPI. As in EhMD simulations, phonon modes are confined to the 10 atoms in the benzene ring for simplicity. Instead of only considering a free molecule as in works done by other groups,[34] here the phonon modes are obtained by solving an extended system containing very long electrodes. The EPI coupling matrices are evaluated through the derivatives of the Fock and overlap matrices with respect to the normal coordinates.[42] All phonon modes are included in our numerical calculations except the one with the lowest frequency, whose characteristic motion time is much longer than that of the electrons and therefore does not affect the transport process of the latter.[43] Actually, in time-dependent simulations where the nuclear motions are restricted to the lowest frequency mode, it is found that the influence of this mode on current is negligible. For time-dependent simulations with phonon self-energy, the bias voltage applied is the same as in previous EhMD simulations. Temperature is set to 300 K for both the electrons in the electrodes and the phonons in the device region.

For steady-state calculations, the phonon self-energy is included at two levels with different accuracy of approximation. Self-consistent Born approximation (SCBA) is an approach that includes the effect of nuclear vibration as self-consistently evaluated self-energies and hence is more accurate. However, it is also more computationally expensive. To reduce the cost, the SCBA self-energy can be approximated by its lowest order expansion (LOE) with respect to coupling strength.[39] Comparison of the currents between different approaches suggests that LOE is good enough for the system of interest. For self-energies due to the electrodes, we adopt the wide-band-limit (WBL) approximation, which assumes that the line width function of the electrode does not change with energy. Steady-state calculations beyond the WBL approximation are also carried out for comparison. In all situations, we confirm that the influence of the nuclear vibration on steady-state current is insignificant. For example, the inclusion of the LOE-type phonon self-energy only slightly enhance the steady current from 1.2 to 2.8 nA. For reference, under the same bias voltage, the steady-state current of the para-linked benzene system is 6400 nA. This conclusion is consistent with ref 34, in which similar results are given by calculations on model system at SCBA level as well as on real system at LOE level. It should be pointed out that destructive interference manifest itself as a transmission dip in the energy gap of the extended π system. Higher bias voltage may get channels far away from the dip involved in the electron transport and weaken the phase cancellation. To prevent this from happening, the bias voltage should be confined to a reasonably low value. Detailed information can be found in the Supporting Information, in which we show that the current of meta-linked benzene system is still three orders of magnitude smaller than that of the para-linked case when bias voltage is raised to 0.5 V.

Figure 3a shows the comparison of the time-dependent currents between the self-energy method (red dotted line) and a typical trajectory from previous EhMD calculations (green line). During the first few femtoseconds, a big surge of the current driven by the bias voltage can be observed in both cases. The overall patterns of the time-dependent currents are quite similar, with only minor difference in their maximum values. After that, the current in the self-energy method reaches its steady state of 2.8 nA in tens of femtoseconds, while it keeps oscillating in the EhMD trajectory. This deviation is caused by the explicit inclusion of nuclear motion in EhMD and the fact that the current in self-energy method is an averaged expectation value. As shown in Figure 2 previously, when statistics are considered, the averaged current of all EhMD trajectories is 1.6 nA, which is still a quite small value compared with the constructive QI case. More interestingly, the times for the currents to reach their maximum values in the two methods are almost the same (~1.3 fs). This is very crucial for the dynamics of the meta-linked benzene system, because it represents the time for charge carriers to travel at the Fermi velocity from the converging point of the two paths to the electrode where measurement takes place.[20] The consistency between the two methods in both steady state and transient dynamics verifies the reliability of our findings in EhMD simulations. Further comparison between the time-dependent current with self-energy of EPI and the one in which the nuclei are fixed shows that the two curves are aligned perfectly with each other, as shown in Figure 3b. The oscillations of currents do not even show any observable phase difference. Therefore, the conclusion can be made that the dynamical features of the QI in meta-linked benzene system are not affected by nuclear vibration either. This will be of great importance in the development of future QuIETs.

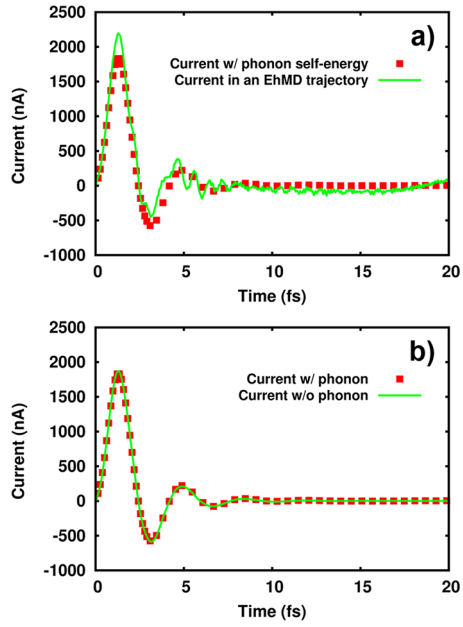

Figure 3. (a) Comparison of the time-dependent currents between the phonon self-energy method (red dotted line) and a typical trajectory from previous EhMD calculations (green line). (b) Time-dependent current through the electrode of the meta-linked benzene system with and without phonon self-energy. The red dotted line represents the current with phonon self-energy, and the green line is the result obtained from calculations with fixed nuclei.

In summary, we use two simulation methods to evaluate the influence of nuclear vibration on electron transport through a meta-linked benzene junction. The results suggest that the destructive QI can still effectively inhibit the electric current in the presence of nuclear vibration at room temperature. Moreover, time-dependent simulations show that QI not only survives the nuclear vibration at steady state but also affects its transient dynamics little. Through exploring the robustness of

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QI against nuclear vibration, we demonstrate the practicability of QuIETs.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpclett.7b02214.

Details of methodology and the steady-state current with different bias voltages for meta- and para-linked benzene systems. (PDF)

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Notes

The authors declare no competing financial interest.

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■ REFERENCES

(1) Aviram, A.; Ratner, M. A. Molecular rectifiers. *Chem. Phys. Lett.* **1974**, *29*, 277−283.

(2) Carroll, R. L.; Gorman, C. B. The Genesis of Molecular Electronics. *Angew. Chem., Int. Ed.* **2002**, *41*, 4378−4400.

(3) Reed, M. A.; Zhou, C.; Muller, C. J.; Burgin, T. P.; Tour, J. M. Conductance of a Molecular Junction. *Science* **1997**, *278*, 252−254.

(4) Joachim, C.; Gimzewski, J. K.; Aviram, A. Electronics Using Hybrid-molecular and Mono-molecular Devices. *Nature* **2000**, *408*, 541−548.

(5) Jauho, A.-P.; Wingreen, N. S.; Meir, Y. Time-dependent Transport in Interacting and Noninteracting Resonant-tunneling Systems. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1994**, *50*, 5528−5544.

(6) Wardrip, A. G.; Mazaheripour, A.; Hüsken, N.; Jocson, J.-M.; Bartlett, A.; Lopez, R. C.; Frey, N.; Markegard, C. B.; Kladnik, G.; Cossaro, A.; et al. Length-Independent Charge Transport in Chimeric Molecular Wires. *Angew. Chem., Int. Ed.* **2016**, *55*, 14267−14271.

(7) Capozzi, B.; Xia, J.; Adak, O.; Dell, E. J.; Liu, Z.-F.; Taylor, J. C.; Neaton, J. B.; Campos, L. M.; Venkataraman, L. Single-molecule Diodes with High Rectification Ratios Through Environmental Control. *Nat. Nanotechnol.* **2015**, *10*, 522−527.

(8) Díez-Pérez, I.; Hihath, J.; Lee, Y.; Yu, L.; Adamska, L.; Kozhushner, M. A.; Oleynik, I. I.; Tao, N. Rectification and Stability of a Single Molecular Diode with Controlled Orientation. *Nat. Chem.* **2009**, *1*, 635−641.

(9) Perrin, M. L.; Burzuri, E.; van der Zant, H. S. J. Single-molecule Transistors. *Chem. Soc. Rev.* **2015**, *44*, 902−919.

(10) Markussen, T.; Stadler, R.; Thygesen, K. S. The Relation between Structure and Quantum Interference in Single Molecule Junctions. *Nano Lett.* **2010**, *10*, 4260−4265.

(11) Rabache, V.; Chaste, J.; Petit, P.; Della Rocca, M. L.; Martin, P.; Lacroix, J.-C.; McCreery, R. L.; Lafarge, P. Direct Observation of Large Quantum Interference Effect in Anthraquinone Solid-State Junctions. *J. Am. Chem. Soc.* **2013**, *135*, 10218−10221.

(12) Mayor, M.; Weber, H. B.; Reichert, J.; Elbing, M.; von Hänisch, C.; Beckmann, D.; Fischer, M. Electric Current through a Molecular Rod—Relevance of the Position of the Anchor Groups. *Angew. Chem., Int. Ed.* **2003**, *42*, 5834−5838.

(13) Guedon, C. M.; Valkenier, H.; Markussen, T.; Thygesen, K. S.; Hummelen, J. C.; van der Molen, S. J. Observation of Quantum Interference in Molecular Charge Transport. *Nat. Nanotechnol.* **2012**, *7*, 305−309.

(14) Fracasso, D.; Valkenier, H.; Hummelen, J. C.; Solomon, G. C.; Chiechi, R. C. Evidence for Quantum Interference in SAMs of Arylethynylene Thiolates in Tunneling Junctions with Eutectic Ga−In (EGaIn) Top-Contacts. *J. Am. Chem. Soc.* **2011**, *133*, 9556−9563.

(15) Arroyo, C. R.; Tarkuc, S.; Frisenda, R.; Seldenthuis, J. S.; Woerde, C. H. M.; Eelkema, R.; Grozema, F. C.; van der Zant, H. S. J. Signatures of Quantum Interference Effects on Charge Transport Through a Single Benzene Ring. *Angew. Chem.* **2013**, *125*, 3234−3237.

(16) Li, Y.; Mol, J. A.; Benjamin, S. C.; Briggs, G. A. D. Interference-based Molecular Transistors. *Sci. Rep.* **2016**, *6*, 33686.

(17) Liu, X.; Sangtarash, S.; Reber, D.; Zhang, D.; Sadeghi, H.; Shi, J.; Xiao, Z.-Y.; Hong, W.; Lambert, C. J.; Liu, S.-X. Gating of Quantum Interference in Molecular Junctions by Heteroatom Substitution. *Angew. Chem., Int. Ed.* **2017**, *56*, 173−176.

(18) Bergfield, J. P.; Heitzer, H. M.; Van Dyck, C.; Marks, T. J.; Ratner, M. A. Harnessing Quantum Interference in Molecular Dielectric Materials. *ACS Nano* **2015**, *9*, 6412−6418.

(19) Solomon, G. C.; Herrmann, C.; Hansen, T.; Mujica, V.; Ratner, M. A. Exploring Local Currents in Molecular Junctions. *Nat. Chem.* **2010**, *2*, 223−228.

(20) Chen, S.; Zhang, Y.; Koo, S.; Tian, H.; Yam, C.; Chen, G.; Ratner, M. A. Interference and Molecular Transport—A Dynamical View: Time-Dependent Analysis of Disubstituted Benzenes. *J. Phys. Chem. Lett.* **2014**, *5*, 2748−2752.

(21) Cardamone, D. M.; Stafford, C. A.; Mazumdar, S. Controlling Quantum Transport through a Single Molecule. *Nano Lett.* **2006**, *6*, 2422−2426.

(22) Markussen, T.; Schiötz, J.; Thygesen, K. S. Electrochemical Control of Quantum Interference in Anthraquinone-based Molecular Switches. *J. Chem. Phys.* **2010**, *132*, 224104.

(23) Koole, M.; Thijssen, J. M.; Valkenier, H.; Hummelen, J. C.; Zant, H. S. J. v. d. Electric-Field Control of Interfering Transport Pathways in a Single-Molecule Anthraquinone Transistor. *Nano Lett.* **2015**, *15*, 5569−5573.

(24) Darwish, N.; Díez-Pérez, I.; Da Silva, P.; Tao, N.; Gooding, J. J.; Paddon-Row, M. N. Observation of Electrochemically Controlled Quantum Interference in a Single Anthraquinone-Based Norbornylogous Bridge Molecule. *Angew. Chem.* **2012**, *124*, 3257−3260.

(25) Sun, L.; Diaz-Fernandez, Y. A.; Gschneidtner, T. A.; Westerlund, F.; Lara-Avila, S.; Moth-Poulsen, K. Single-molecule Electronics: From Chemical Design to Functional Devices. *Chem. Soc. Rev.* **2014**, *43*, 7378−7411.

(26) Jia, C.; Guo, X. Molecule−electrode Interfaces in Molecular Electronic Devices. *Chem. Soc. Rev.* **2013**, *42*, 5642−5660.

(27) Guo, X.; Small, J. P.; Klare, J. E.; Wang, Y.; Purewal, M. S.; Tam, I. W.; Hong, B. H.; Caldwell, R.; Huang, L.; O'Brien, S.; et al. Covalently Bridging Gaps in Single-Walled Carbon Nanotubes with Conducting Molecules. *Science* **2006**, *311*, 356−359.

(28) Tao, N. J. Electron Transport in Molecular Junctions. *Nat. Nanotechnol.* **2006**, *1*, 173−181.

(29) Arroyo, C. R.; Tarkuc, S.; Frisenda, R.; Seldenthuis, J. S.; Woerde, C. H. M.; Eelkema, R.; Grozema, F. C.; van der Zant, H. S. J. Signatures of Quantum Interference Effects on Charge Transport Through a Single Benzene Ring. *Angew. Chem., Int. Ed.* **2013**, *52*, 3152−3155.

(30) Hihath, J.; Bruot, C.; Tao, N. Electron−phonon Interactions in Single Octanedithiol Molecular Junctions. *ACS Nano* **2010**, *4*, 3823−3830.

(31) Gaudioso, J.; Lauhon, L. J.; Ho, W. Vibrationally Mediated Negative Differential Resistance in a Single Molecule. *Phys. Rev. Lett.* **2000**, *85*, 1918−1921.

DOI: 10.1021/acs.jpclett.7b02214
J. Phys. Chem. Lett. 2017, 8, 5166−5170

(32) Kushmerick, J. G.; Lazorcik, J.; Patterson, C. H.; Shashidhar, R.; Seferos, D. S.; Bazan, G. C. Vibronic Contributions to Charge Transport Across Molecular Junctions. *Nano Lett.* **2004**, *4*, 639−642.
(33) Ballmann, S.; Härtle, R.; Coto, P. B.; Elbing, M.; Mayor, M.; Bryce, M. R.; Thoss, M.; Weber, H. B. Experimental Evidence for Quantum Interference and Vibrationally Induced Decoherence in Single-Molecule Junctions. *Phys. Rev. Lett.* **2012**, *109*, 056801.
(34) Markussen, T.; Thygesen, K. S. Temperature Effects on Quantum Interference in Molecular Junctions. *Phys. Rev. B: Condens. Matter Mater. Phys.* **2014**, *89*, 085420.
(35) Zhang, Q. *A Theory of Ehrenfest Dynamics for Open Systems and Its Applications*. Dissertation, The University of Hong Kong, Pokfulam, Hong Kong, 2015.
(36) Kwok, Y. H.; Xie, H.; Yam, C. Y.; Zheng, X.; Chen, G. H. Time-dependent Density Functional Theory Quantum Transport Simulation in Non-orthogonal Basis. *J. Chem. Phys.* **2013**, *139*, 224111.
(37) Zheng, X.; Chen, G.; Mo, Y.; Koo, S.; Tian, H.; Yam, C.; Yan, Y. Time-dependent Density Functional Theory for Quantum Transport. *J. Chem. Phys.* **2010**, *133*, 114101.
(38) Zheng, X.; Wang, F.; Yam, C. Y.; Mo, Y.; Chen, G. Time-dependent Density-functional Theory for Open Systems. *Phys. Rev. B: Condens. Matter Mater. Phys.* **2007**, *75*, 195127.
(39) Zhang, Y.; Yam, C. Y.; Chen, G. Dissipative Time-dependent Quantum Transport Theory. *J. Chem. Phys.* **2013**, *138*, 164121−164121.
(40) Zhang, Y.; Yam, C.; Chen, G. Dissipative Time-dependent Quantum Transport Theory: Quantum Interference and Phonon Induced Decoherence Dynamics. *J. Chem. Phys.* **2015**, *142*, 164101−164101.
(41) Ke, S.-H.; Yang, W.; Baranger, H. U. Quantum-inteference-controlled Molecular Electronics. *Nano Lett.* **2008**, *8*, 3257−3261.
(42) Pecchia, A.; Di Carlo, A.; Gagliardi, A.; Sanna, S.; Frauenheim, T.; Gutierrez, R. Incoherent Electron−Phonon Scattering in Octanethiols. *Nano Lett.* **2004**, *4*, 2109−2114.
(43) Lindsay, S. M.; Ratner, M. A. Molecular Transport Junctions: Clearing Mists. *Adv. Mater.* **2007**, *19*, 23−31.

DOI: 10.1021/acs.jpclett.7b02214
J. Phys. Chem. Lett. 2017, 8, 5166−5170