Real-Time Atomistic Dynamics of Energy Flow in an STM Setup: Revealing the Mechanism of Current-Induced Molecular Emission

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Supporting Information

ABSTRACT: Detailed understanding of the current-induced fluorescence mechanism constitutes an exciting challenge as it can open the way to efficient coupling between an electric field and light at the nanoscale. At the same time, a number of published experimental studies give an unclear, contradictory picture of this phenomenon working principle. Here, for a system consisting of a silver tip and a porphyrin molecule, we perform for the first time fully atomistic, real-time nonadiabatic dynamics simulations to study the process of energy transfer and relaxation in an STM setup. We calculate time scales of all crucial processes and explain their atomic details. On this basis, we confirm and characterize the dual mechanism of the observed emission based on competing elastic and inelastic electron transfer between the metal tip and the molecule.

Scanning tunneling microscopy (STM), since its beginnings in the early 1980s,1,2 has evolved into a powerful tool for probing and controlling single atoms and molecules on conductive surfaces. Aside from its original applications (subnanoscale visualization and physical manipulation at the atomic level), it has further opened the way for modern techniques and emerging technologies based on single-molecule electrically operated units, including molecular junctions and transistors,3–10 current- and electric field-controlled molecular switches,11–16 and nano-optoelectronic molecular devices.17–21

The mechanisms of the multiple processes taking place during STM measurements are quite complex and involve multiple steps happening at the nanoscale, with energy and charge evolution playing central roles. Deep understanding of these processes leaves a lot of open questions that, if cleared, could assist in taking full advantage of the STM technique. An accurate theoretical description of the complex STM working principles is highly challenging as it requires joining fundamental macroscopic and microscopic concepts from chemistry and physics.22

The experimental work by Qiu et al.23 reported for the first time a sharp current-induced emission from a single magnesium porphine molecule and identified the observed luminescence as being of dual, plasmonic, and molecular origin. At the same time, they reported negative charge of the emitting molecular unit. On the other hand, Chen et al.26 ascribed measured current-induced emission in the very same system to purely molecular fluorescence from a neutral center. Baker and Kirczenow28 investigated theoretically possible molecular emission mechanisms in the setup originally used by Qiu et al.23 Focusing on molecular emission and omitting the possibility of plasmonic emission, they applied a local-electrode model with a continuous wave current representation and proposed an explanation for the varying emission patterns depending on the molecule configuration. Despite the efforts taken, still a number of contradictory findings have not been resolved, which, aside from the original problem with the electron transfer mechanism, include questions about the charge of the molecular unit under short-circuit conditions and explanation of the complex response of the recorded emission spectrum to the changing bias.

In this Letter, we for the first time employ fully atomistic, nonadiabatic molecular dynamics (NAMD) to simulate directly in the time domain the mechanisms of charge injection and energy relaxation within the tip and emitting molecule. In addition to the overall picture of the current-induced emission, our approach allows for identification of the key steps of the energy evolution and their time scales. We find that the elastic electron transfer followed by the nonradiative induced emission from a single magnesium porphine molecule and identified the observed luminescence as being of dual, plasmonic, and molecular origin. At the same time, they reported negative charge of the emitting molecular unit. On the other hand, Chen et al.26 ascribed measured current-induced emission in the very same system to purely molecular fluorescence from a neutral center. Baker and Kirczenow28 investigated theoretically possible molecular emission mechanisms in the setup originally used by Qiu et al.23 Focusing on molecular emission and omitting the possibility of plasmonic emission, they applied a local-electrode model with a continuous wave current representation and proposed an explanation for the varying emission patterns depending on the molecule configuration. Despite the efforts taken, still a number of contradictory findings have not been resolved, which, aside from the original problem with the electron transfer mechanism, include questions about the charge of the molecular unit under short-circuit conditions and explanation of the complex response of the recorded emission spectrum to the changing bias.

In this Letter, we for the first time employ fully atomistic, nonadiabatic molecular dynamics (NAMD) to simulate directly in the time domain the mechanisms of charge injection and energy relaxation within the tip and emitting molecule. In addition to the overall picture of the current-induced emission, our approach allows for identification of the key steps of the energy evolution and their time scales. We find that the elastic electron transfer followed by the nonradiative

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energy relaxation within the molecule outcompetes all of the alternative relaxation paths in terms of rate and efficiency, but the inelastic electron path involving tip plasmonic states leads to more efficient fluorescence, which eventually, for a sufficiently large applied voltage, results in a mixed-mechanism emission. The sharp and wide peaks in the recorded emission spectra are attributed to molecular and plasmonic emission, respectively, and their previously unclear sensitivity to bias applied between the tip and the source electrode is explained. The provided atomistic insights can assist in optimal design of emerging nano-optoelectronic devices operating on single molecules, such as plasmon-generating field-effect transistors or light-emitting diodes.

We employ the plane-wave density functional theory approach, as implemented in the QUANTUM ESPRESSO package, to describe electronic properties of the system including a silver tip represented by the Ag$_{80}$ tetrahedral cluster and a Zn(II)-etioporphyrin I molecule, following the original setup used in the experiment by Qiu et al. The Ag$_{80}$ representation of the STM tip provides a practical compromise between accuracy and computational efficiency. The small cluster underestimates the density of tip states and overestimates the energies of the lowest states contributing to the plasmon resonance. As a result, the contribution of the plasmonic energy transfer mechanism is likely underestimated in our simulations. The system’s structure was optimized in two steps: first, the geometry of the isolated molecule was optimized at the PBE functional, with the kinetic energy cutoff for the wave function and charge density set to 60 and 800 Ry, respectively, and with the Grimme’s DFT-D2 dispersion correction included. At this stage, the molecule–tip distance was set to 6 Å, in accordance with the original experimental study. Figure 1a shows the optimized structure of the system. The Cartesian coordinates can be found in Table S1 in the Supporting Information (SI).

Figure 1. (a) Side and top views of the geometric structure of the studied system consisting of a silver tip and the porphyrin molecule. (b) Scheme of the considered current-induced emission mechanisms. The two sets of arrows show different paths for the possible light emission: black — elastic electron injection from the tip to a molecular excited state, followed by nonradiative relaxation to the lowest molecular excited state and the molecular emission; red — inelastic electron tunneling from the tip into the molecular ground state, simultaneously accompanied by plasmonic emission.

The same electronic structure settings were used during the 500 fs thermalization dynamics, performed at 300 K with the Andersen thermostat. Subsequently, a 500 fs microcanonical trajectory was generated and used to sample initial conditions for the extended 10 ps nonadiabatic dynamics study with a time step of 1 fs. The NAMD calculations were performed using the Decoherence Induced Surface Hopping (DISH) approach, implemented with the PYXAID code under the classical path approximation. The results were averaged over 500 initial conditions, each of them involving 200 realizations of the stochastic surface hopping process, to achieve high-quality time scale estimations. The atomic structure and orbital visualizations were prepared with the XCRYSDEN software.

The nonradiative relaxation time scales ($\tau_{\text{dip}}, \tau_{\text{cool}}, \tau_{\text{rel}}$) were obtained from an exponential fit to the population change. The reported pure-dephasing times ($\tau_{\text{dip}}$), measuring the rate at which phases of nonadiabatically coupled states decohere in time, were calculated using the second-order cumulant approximation to the optical response function. The radiative relaxation lifetimes ($\tau_{\text{f}}$) were determined using the Einstein coefficients for spontaneous transition as $\tau_{\text{f}} = \text{const.}/(\nu f)$, where $\nu$ is the transition energy, $f$ is transition oscillator strength, and const. = $m_e c^2/((16\pi\epsilon^2)$ with $c$, $m_e$ and $\epsilon$ corresponding to light speed in vacuum, electron mass, and electron charge, respectively.

Figure 1b schematically shows the energy levels alignment in the system. Starting from the tip side (left in the picture), one finds a dense manifold of states forming the valence (VB$_{Ag}$) and the conduction bands (CB$_{Ag}$) of the silver tip. These levels couple through a vacuum gap with the molecular orbitals of the porphyrin unit. The energy levels of the tip and the molecule constitute together the active space for the performed calculations. To gain a broader perspective, we also included in the scheme in Figure 1b an insulating oxide layer (Ox.) and the metal electrode as they were present in the experiment. In our study, however, we did not explicitly include the insulating and metal electrode components. Our choice of the explicitly treated system components is based on the nature of the phenomenon of interest, that is, the mechanism of the current-induced emission. According to the experimental findings reported in the original paper, the emission can solely occur between the tip and molecular states or within the molecule.
alone due to tested strong screening of the other metal electrode. Thus, the electrode and oxide electronic levels do not contribute explicitly to the emission mechanism. At the same time, their indirect role remains important in two other aspects. First, the oxide generally weakens the coupling between the molecular levels and electrode, making the emission from the molecule possible; otherwise, it would be quenched. This decoupling effect supports isolation of the tip and the molecule from the electrode in our simulations. Second, the oxide layer and the electrode together participate in the voltage drop within the whole studied setup, giving quantitative reference for translating applied bias to excess energy available for light emission. Thus, their omission makes the reference point uncertain. At the same time, however, the energy of the top of their valence bands is limited by the molecular HOMO energy because any emission involving the HOMO orbital is only possible with its partial depopulation. This imposes a lower bound for the voltage needed to access the particular excess energy. All of the reported applied voltage values should be thus interpreted in this lower-bound sense.

The application of voltage causes major changes in the system’s electronic configuration. First, the initially populated energy levels coupled to the negative pole of the bias source start accepting incoming electrons (silver tip), while the originally populated levels coupled to the positive pole start to get depleted (metal electrode). Eventually, the molecular orbitals interacting with both contacts may also change their electronic populations according to the strength of their individual electronic couplings. Under certain conditions, this charge flow may result in current-induced light emission, which can be associated with different energy flow mechanisms, schematically shown in Figure 1b. Depicted with the black set of arrows is a path involving elastic injection of the electron from the tip to the molecule, followed by intramolecular relaxation and final radiative transition between the molecular HOMO and LUMO. Alternatively, as marked with the red set of arrows, a spatially extended tip state (most likely of plasmonic nature) may directly couple to the depopulated molecular HOMO, and upon inelastic electron hopping, a photon could be emitted. Other possible emission options, such as plasmonic emission solely involving the tip and electrode states, have been excluded by the experimental study in this case.28 The other possible consequence of the applied voltage is a shift of the energy levels positions and their further relaxation due to the electron transfer. These effects have not been included in the present study as they should be primarily limited to a linear correction to the absolute energy levels,28 having minor impact on the established energy flow mechanism.

Next, consider in more detail the system’s electronic structure. Figure 2 shows the calculated electronic density of states (DOS) projected over the molecular and silver tip units. The dense manifold of unoccupied tip orbitals embeds a doubly degenerate molecular LUMO, while the HOMO, also centered at the molecule, lies within the silver–nanoparticle bandgap. At this moment, it should be stressed that the exact energies of the molecular levels with respect to the metal particle background must be treated with caution as they may show dependence on the chosen methodological settings. Nonetheless, the presented energy level alignment sets a good base for further understanding of the physics behind the charge and energy transfer processes under investigation. At the same time, comparison with available experimental and higher level theoretical data confirms reasonably good quality of the calculated energy features for the silver cluster45,44 and higher levels of the porphyrin.35,46 The HOMO–LUMO energy difference of the porphyrin unit shows critical dependence on the computational crystal cell size and was found to be underestimated47,48 at the applied level of theory. For that, this value was later on scaled up in accordance with the experimentally measured absorption onset to 2 eV, for the purpose of radiative lifetime calculations. Because electrons are transferred from the tip, through the molecule, to the substrate, the Fermi energy of the tip increases when voltage is applied to the system. The originally empty tip states get populated, while the states on the electrode side are depopulated. The opening energy window sets the limit over possible electronic radiative transitions within the molecule. Knowing the calculated DOS pattern and the range of voltage values applied in the experiment (up to 2.4 V),23 we therefore conclude that, for energetic reasons, the molecular emission should be most probably associated with the HOMO–LUMO transition (neutral emission) and not transition between the LUMO and LUMO+1 (anionic emission) as the LUMO+1 level cannot be populated at biases below 3.8 V.

Figure 3 visualizes the orbitals crucial for the present study, numbered with respect to the HOMO with rising energy. Please refer to Figure S1 in the SI for visualization of the higher-energy orbitals and the top-view pictures. While the HOMO (0) orbital shows important contributions from the metal center and complexing nitrogen atoms, both LUMOs, LUMO (4) and LUMO+1 (5), are built from the π carbon orbitals. This observation, suggesting weak oscillator strength for the HOMO–LUMO transition, stays in agreement with the experimentally recorded low intensities of the lowest-energy transitions in porphyrin–metal complexes.47,48 Another interesting feature is the presence of an orbital delocalized over the tip and molecule (6), energetically lying just over the LUMOs. Its nature comes from strong interaction between the tip and porphyrin, and its delocalization extent is expected to vary with the distance between both units.

In addition to the orbitals pictures, Figure 3 summarizes all charge and energy transfer processes investigated in the present contribution. On the one hand, the NAMD simulations account for the total charge evolution mechanism induced in the tip and molecule system by the applied voltage (transitions 7−...−4−0). On the other hand, the simulations
also provide details on the individual evolution steps. First, the electron injection from the tip to the molecule is separately analyzed (transitions from levels 9–7 to 6). Then electron relaxation within the molecular unit (transition 6–5–4) is investigated. Finally, the charge recombination (transition 4–0) is studied. Further, an alternative path involving direct, inelastic electron transfer between lower tip states and the HOMO is also modeled (3–1 to 0). For each of the steps, we determine characteristic lifetimes and identify leading degrees of freedom facilitating the particular nonadiabatic transition. The numeric values of all crucial factors discussed in the course of the analysis are gathered in Tables 1 and 2. Facilitating comparison with experiment, it is important to point out that plasmons typically show broad emission peaks, while molecules are characterized by much sharper emission peaks.

Starting from a broad perspective, Figure 4a,b presents the overall evolution of the electronic populations in response to the applied bias. The initially populated orbital (7) is the

Table 1. Electronic State Population Dynamics for the Elastic Electron Injection Mechanism

<table>
<thead>
<tr>
<th>Injection</th>
<th>Initial Orbital (x)</th>
<th>$\Delta E_{x-0}$ (eV)</th>
<th>NACI$_{(x-0)}$ (meV)</th>
<th>$\tau_{\text{deph}(x-0)}$ (fs)</th>
<th>$\tau_{\text{inj}(x-0)}$ (ps)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9 [1.90]</td>
<td>0.15</td>
<td>3.6</td>
<td>45</td>
<td>3.85</td>
<td></td>
</tr>
<tr>
<td>8 [1.85]</td>
<td>0.13</td>
<td>2.4</td>
<td>70</td>
<td>4.29</td>
<td></td>
</tr>
<tr>
<td>7 [1.75]</td>
<td>0.09</td>
<td>2.1</td>
<td>65</td>
<td>5.69</td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Electronic State Population Dynamics for the Inelastic Electron Tunneling Mechanism

<table>
<thead>
<tr>
<th>Inelastic Tunneling</th>
<th>Initial Orbital (x)</th>
<th>$\Delta E_{x-0}$ (eV)</th>
<th>NACI$_{(x-0)}$ (meV)</th>
<th>$\tau_{\text{deph}(x-0)}$ (fs)</th>
<th>$\tau_{\text{inj}(x-0)}$ (ps)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 [0.90]</td>
<td>0.79</td>
<td>0.3</td>
<td>7</td>
<td>&gt;3.3</td>
<td></td>
</tr>
<tr>
<td>2 [0.75]</td>
<td>0.71</td>
<td>0.2</td>
<td>7</td>
<td>&gt;5.2</td>
<td></td>
</tr>
<tr>
<td>1 [0.70]</td>
<td>0.69</td>
<td>0.2</td>
<td>7</td>
<td>&gt;6.5</td>
<td></td>
</tr>
</tbody>
</table>

"Initial orbital: starting orbital in the surface hopping simulation; $\Delta E$: energy difference between the chosen pair of orbitals; NACI: time-averaged absolute value of the nonadiabatic coupling between the chosen pair of states; $\tau_{\text{deph}}$: pure-dephasing time; $\tau_{\text{inj}}$: characteristic time scale for the inelastic electron injection.

lowest possible pure-tip level lying over the unoccupied molecular orbitals, and its energy with respect to the Fermi level corresponds in our calculation to an applied voltage of roughly 1.75 V. This threshold voltage is strictly required to initiate the analyzed energy relaxation path because the unoccupied molecular levels are not accessible for lower biases. Figure 4a demonstrates a quick, picosecond time scale population decay of the starting state, followed by an even faster conversion within the 6–5–4 molecule-centered states. At the same time, when molecular LUMO (4) is reached, further electronic population flow to the ground state (HOMO) is strongly suppressed, as shown in Figure 4b, due to small overlap between the LUMO and HOMO, localized in different regions of the porphyrin system.

After this general overview of the process dynamics, we now move to a detailed analysis of its identified crucial steps: electron injection, electron cooling, and nonradiative relaxation to the ground state. Figure 4c shows how increasing the voltage applied between the tip and the electrode affects the rate of electronic population flow from the tip to the molecule. Higher voltage values activate higher-energy tip levels to participate in the electron transfer process, which we model with a series of surface hopping simulations starting with single-electron occupation at these newly accessed levels. In result, we observe a ca. 50% increase of the electron injection rate as the applied bias rises from 1.75 to 1.90 V (see Table 1).
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In the next step of the dynamic evolution, an electron injected to the molecule undergoes rapid cooling, driving it down to the molecular LUMO. To get a direct measure of the cooling time scale, we performed a separate surface hopping study, in which the dynamics started from the molecular state populated in the injection step, orbital 6. The cooling time scale, calculated from the LUMO population rise, was estimated at ≈0.6 ps, making cooling the fastest process observed in the study. This rapid intramolecular relaxation gives an explanation for the sharp emission energy cutoff found in the experiment as the subpicosecond transition time scale leaves no time for the fluorescence emission from states other than the LUMO, in accordance with Kasha’s rule. A look over the cooling power spectra allows again identification of atomic vibrations contributing the most to the energy relaxation dynamics. In this case, three important energy regions have been distinguished: \( \nu < 200 \text{ cm}^{-1} \), corresponding to the silver pyramid stretching; \( 1200 < \nu < 1400 \text{ cm}^{-1} \), involving pyrrole ring deformations; and \( 2500 < \nu < 3000 \text{ cm}^{-1} \), assigned primarily to C–H stretching in the large-ring porphyrin framework. The latter were found especially important for facilitating the transition between LUMO (4) and its quasi-degenerate partner state (5). Please refer to Figure S2 in the SI for plots of power spectra and state population dynamics.

Once the cooling is completed, the nonradiative deactivation process is expected to compete with the possible radiative molecular emission. The charge-recombination surface hopping study, including the HOMO and LUMO, gave a nonradiative recombination time of \( \tau_{\text{nr}} \approx 290 \text{ ps} \). We find that the whole-porphyrin stretching and pyrrole deformation modes almost equally participate in the process. The long nonradiative lifetime originates from the ultrafast loss of quantum coherence on the one hand and from small nonadiabatic coupling on the other hand (see Table 1). To get a notion of how this could affect the molecular fluorescence emission, we estimated the radiative recombination lifetime, \( \tau_r \approx 6620 \text{ ns} \). This value, several orders of magnitude larger than the estimated nonradiative lifetime, suggests a rather weak molecular radiative emission in the studied STM–porphyrin system.

Finally, to test the hypothesis of the alternative, plasmon-assisted emission mechanism, we modeled the nonradiative electron transfer dynamics in the low-voltage regime. In analogy to the elastic electron injection step, we estimated the nonradiative lifetimes for electrons being independently transferred from all available low-energy tip orbitals (1–3). We found that in all cases the process is strongly suppressed by a combination of ultrafast decoherence and very small nonadiabatic coupling values. The nonradiative electron injection rates lie in the nanosecond regime, as shown in Table 2. At the same time, the calculated fluorescence lifetimes range from 730 to 40 ns, for an applied voltage of 0.7–0.9 V, respectively. Thus, one may consider the plasmon-assisted emission path as a possible mechanism of the observed current-induced emission, which agrees well with the wide, lower-energy peaks recorded in the experiment. This interpretation also supports the shift of the high-energy cutoff observed with increasing voltage in the case of the low-bias peaks as even a small voltage change leads to activation of new, densely lying tip electronic levels in the inelastic electron transition scenario.

Figure 4. (a,b) Electronic population dynamics of the system along the elastic electron injection path; (c) voltage-dependent dynamics of charge injection to molecular state 6 and (d) power spectrum for the voltage-dependent injection processes shown on the background of the system’s vibrational modes (thin gray lines). The numbers 1.75, 1.85, and 1.90 in (c,d) represent the applied bias in volts. For state numbering in (a,b), refer to Figure 3, and for that in (c,d), refer to Table 2.

This rate increase can explain why in the experiment Qiu et al. observed rising intensity of sharp emission spectral peaks as they were increasing the applied voltage. Further, Figure 4d identifies the system’s vibrations that facilitate the electron injection most efficiently. The shown power spectra illustrate interactions between delocalized, top molecular orbital (6), and electron-donating tip orbitals (7, 8, and 9). In all cases, the strongest impact comes from the low-energy vibrations (\( \nu < 200 \text{ cm}^{-1} \)), corresponding to Ag-pyramid breathing modes and its quasi-degenerate partner state (5). Please refer to Figure S2 in the SI for plots of power spectra and state population dynamics.
Taking into account the experimental current of 0.5 nA, one estimates that an electron spends about $10^{-10}$ s on the molecule. The injection and cooling processes are predicted to occur on much faster time scales, on the order of a single ps. The nonradiative recombination within the molecule, setting an effective limit over the molecular emission lifetime, falls in the range of a few hundred, which is similar to the estimated electron residence time. The plasmon-related time scales exceed this limit approximately by 1 order of magnitude. Therefore, the probability of the plasmon-related emission is small but not zero. At the same time, the small representation of the tip underestimates the DOS contributing to the plasmon resonance, and therefore, the importance of the plasmon pathway to emission should be higher in the realistic system.

In conclusion, by means of time domain nonadiabatic molecular dynamics, we studied the mechanism of energy evolution in an STM setup coupled to a chromophore molecule, with a purpose of explaining unresolved doubts about the exact mechanism of the experimentally observed current-induced light emission. We found that once the threshold applied voltage is reached, fast and efficient electron transfer from a metal tip to unoccupied molecular states takes place. This is followed by ultrafast internal energy relaxation within the molecule, eventually resulting in population of the molecular LUMO on a picosecond time scale after the initial bias application. From that point, a competition between nonradiative and radiative relaxation processes leads to weak molecular fluorescence with a sharp high-energy cutoff. At the same time, we found that the slow inelastic electron transfer from low-energy tip states constitutes the source of the wideband light emission observed for low biases. Finally, we attribute the experimentally recorded sharp peak rise in the emission spectrum in response to increasing voltage to enhanced elastic electron transfer between the tip and unoccupied molecular orbitals. The reported analysis indicates dual, molecular, and plasmonic character of the current-induced fluorescence observed from the STM setup containing the porphyrin molecule. The atomistic insights into the mechanism of charge and energy evolution in such hybrid molecular-metallic, electrically controllable systems can open new possibilities for optimal design of emerging nano-optoelectronic molecular devices.

**ASSOCIATED CONTENT**

* Supporting Information
The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpcllett.8b01331.

Atomic coordinates, molecular orbitals visualization, power spectrum, and population dynamics for intramolecular electron cooling (PDF)

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**Notes**
The authors declare no competing financial interest.

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