Photoinduced dynamics and nonequilibrium characteristics in quasi-one-dimensional electron systems: Mott insulators vs. band insulators

Kenji Yonemitsu

*Institute for Molecular Science, Okazaki 444-8585, Japan*

*Graduate University for Advanced Studies, Okazaki 444-8585, Japan*

E-mail: kxy@ims.ac.jp

**Abstract.** Electron-electron interactions play an important role in nonequilibrium properties of molecular materials. First, we show differences between photoinduced ionic-to-neutral and neutral-to-ionic transitions in quasi-one-dimensional extended Peierls Hubbard models with alternating potentials. Cooperative dynamics lead to nonlinear ionicity in the former, while uncooperative dynamics lead to quite linear ionicity in the latter, as a function of the energy supplied from the oscillating electric field. Interchain electron-electron interactions bring about initial competition among metastable and stable domains in neighboring chains, slowing down the phase transition. Interchain elastic couplings are necessary to form a ferroelectric long-range order. Second, we show differences between field-effect characteristics of Mott insulators and those of band insulators in one-dimensional Hubbard models, to which tight-binding models are attached for metallic electrodes and scalar potentials are added for interfacial barriers. Ambipolar characteristics are found in the former, while unipolar characteristics generally appear in the latter. In the former, charge transport is cooperative so that the drain current is insensitive to the difference between the work function of the channel and that of the electrodes, and thus insensitive to the polarity of the gate bias.

1. Introduction

Many molecular materials have strong anisotropy in electronic conduction owing to their molecular arrangements in the crystals. In addition, electron correlations also contribute to the low-dimensional motion of carriers [1]. Some of their intriguing properties are observed in nonequilibrium conditions. Photoinduced phase transitions [2] are among them, to which the cooperativity in interacting electron systems is crucial. In the mixed-stack organic charge-transfer complex, TTF-CA (TTF=tetrathiafulvalene, CA=chloranil), charge-transfer strings are photogenerated and bring about neutral-ionic transitions [3]. The cooperativity is manifested by a threshold intensity of excitation [4], coherent motion of macroscopic domain boundaries [5], and self-organized long-range ferroelectric order [6, 7]. Recent experiments show different cooperativity between the ionic-to-neutral and the neutral-to-ionic transitions [8]. We theoretically study how different they are. It is suggested to be important that the ionic state is a Mott insulator while the neutral state is a band insulator.

Field-effect transistors are fabricated on many molecular materials. Recently, ambipolar field-effect characteristics are reported in metal-insulator-semiconductor field-effect transistor
\[ H_{PH} = \sum_{l=1}^{L} \left( \sum_{j=1}^{M} H_{l,j} + \sum_{j=1}^{M-1} H_{l,j,j+1} \right) \]

\[ H_{l,j} = -t_0 \sum_{\sigma} \left( c_{l,j,\sigma}^\dagger c_{l+1,j,\sigma} + c_{l+1,j,\sigma}^\dagger c_{l,j,\sigma} \right) + (-1)^l \frac{d}{2} n_{l,j} + U n_{l,j,\uparrow} n_{l,j,\downarrow} \]

\[ + \tilde{V}_{l,j} \delta n_{l,j} \delta n_{l+1,j} + \frac{k_1}{2} \tilde{y}_{l,j}^2 + \frac{k_2}{4} \tilde{u}_{l,j}^4 + \frac{m_{l,j}}{2} \ddot{u}_{l,j}^2, \]

\[ H_{l,j,j+1} = U_{\perp} \delta n_{l,j} \delta n_{l+1,j} + V_{\perp} \delta n_{l,j} \delta n_{l+1,j} + V_{\perp 2} \delta n_{l,j} \delta n_{l+1,j+1} + \frac{k_{1\perp}}{2} (u_{l,j+1} - u_{l,j})^2, \]

where, \( c_{l,j,\sigma}^\dagger (c_{l,j,\sigma}) \) is the creation (annihilation) operator of an electron with spin \( \sigma \) at site \( l \) of chain \( j \). \( n_{l,j,\sigma} = c_{l,j,\sigma}^\dagger c_{l,j,\sigma} \). \( \delta n_{l,j} = n_{l,j,\uparrow} + n_{l,j,\downarrow} \). \( \tilde{V}_{l,j} \delta n_{l,j} \delta n_{l+1,j} \) depends on the bond length \( y_{l,j} \), \( \tilde{V}_{l,j} = V + \beta_2 y_{l,j}^2 \), where \( V \) is for the regular lattice. The parameter \( t_0 \) denotes the nearest-neighbor transfer integral, \( d \) the level difference between the neighboring orbitals in the neutral limit, and \( U \) the on-site repulsion strength. The elastic energy is expanded up to the fourth order with the parameters \( k_1 \) and \( k_2 \). The quantity \( m_{l,j} \) denotes the molecular mass. The interchain interactions are characterized by the repulsion strengths \( U_{\perp}, V_{\perp 1}, V_{\perp 2} \) for neighboring molecules, and the elastic constant \( k_{1\perp} \). The number of sites in a periodic chain is denoted by \( L \), and that of chains by \( M \).

We numerically solve the time-dependent Schrödinger equation within the unrestricted Hartree-Fock (HF) approximation for the electronic part and the classical equation of motion for the lattice part. Random numbers are added to the initial lattice variables according to the Boltzmann distribution at a fictitious temperature \( T \). Photoexcitations are introduced by modifying the transfer integral with the Peierls phase as explained in [12]. We use \( M=10 \) chains of \( L=100 \) sites, \( t_0=0.17eV, U=1.528eV, V=0.604eV \) (when the ionic phase is photoexcited) or \( V=0.600eV \) (when the neutral phase is photoexcited), \( \beta_2=8.54eV, k_1=4.86eV, k_2=3400eV \) [10], and the bare phonon energy \( \omega_{\text{opt}}=0.0192eV \) [11]. The parameter \( d \) is set at 2.716eV for (MISFET) device structures based on organic single crystals of the quasi-one-dimensional Mott insulator (BEDT-TTF)(F\(_2\)TCNQ) [BEDT-TTF=bis(ethylenedithio)tetrathiafulvalene, F\(_2\)TCNQ=2,5-difluorotetracyanoquinodimethane] [9]. In quasi-one-dimensional systems with coherent band transport, the insulator-electrode interface barrier potentials are crucial to the current-voltage characteristics. As long as the work functions of the electrodes are different from that of the channel, the characteristics are usually expected to be asymmetric with respect to the polarity of the gate bias. Thus band insulators show unipolar characteristics. The ambipolar characteristics of the organic Mott insulator imply very similar effects of the insulator-electrode interface barrier potentials, when combined with electron correlation effects, for electron and hole injections. We theoretically show that the ambipolar characteristics of Mott insulators are due to cooperativity originating from electron-electron interactions.

2. Photoinduced neutral-ionic transitions in mixed-stack charge-transfer complexes

In order to study the photoinduced phase transitions in the TTF-CA complex, we add interchain electron-electron and elastic couplings to the one-dimensional extended Peierls-Hubbard model with alternating potentials for the highest occupied molecular orbital (HOMO) at the donor site and the lowest unoccupied molecular orbital (LUMO) at the acceptor site [10, 11],

\[ \omega_{\text{opt}}=0.0192eV \] [11]. The parameter \( d \) is set at 2.716eV for
$U_{\perp}=V_{\perp,1}=V_{\perp,2}=0$ [10], and it is so varied that the difference between the total energy of the neutral phase and that of the ionic phase is unchanged when the interchain electron-electron interactions are introduced. The electric field used here is $E(t) = E_{\text{ext}} \sin \omega_{\text{ext}} t$ with amplitude $E_{\text{ext}}$ and frequency $\omega_{\text{ext}}$ for $0 < t < 2\pi N_{\text{ext}}/\omega_{\text{ext}}$ with integer $N_{\text{ext}}$. $E(t)$ is zero otherwise. The ionicity is defined as $\rho = 1 + 1/(LM) \sum_{l=1}^{L} \sum_{j=1}^{M} (-1)^l (n_{l,j})$. The single-chain results are first summarized before the effects of the interchain couplings are discussed.

2.1. Difference of ionic-to-neutral and neutral-to-ionic transitions

When the dimerized ionic phase is photoexcited, a sufficiently strong or long pulse can achieve the transition into the neutral phase with equidistant molecules [12]. The threshold behavior is observed by plotting the final ionicity as a function of the increment of the total energy. The threshold value is almost independent of whether the field strength is varied or the pulse duration is varied, and of whether the frequency of the electric field is on resonance or off resonance with the excitonic linear-absorption peak. When the very weak field is applied for long, however, the supplied energy dissipates more into ionic-anti-ionic solitons reducing the ferroelectric order before the transition. Then the correlation between the electronic dynamics and the lattice dynamics becomes weak. In such a case, the threshold absorption is shifted to a larger value because the supplied energy is not directly used to transfer charge density along the chain.

Below the threshold absorption, the photoirradiation does not largely change the electronic system including the ionicity, although the phases of the staggered lattice displacements are generally disordered. Above the threshold absorption, a neutral domain is created somewhere in a stochastic manner due to the initial lattice fluctuations, and it spontaneously grows (figure 1) even without energy supply from the electric field. The manner in which neutral domains are created and their initial growth in multi-chain systems are modified by the interchain electron-electron interactions, as shown below. In the figures shown here and below, the electric field of $eaE_{\text{ext}}/\omega_{\text{opt}}=3$ and $\omega_{\text{ext}}/\omega_{\text{opt}}=28$ is continuously applied to the states, which initially have $T/t=10^{-3}$. The staggered lattice displacement $u_{\text{st},l,j}$ is defined as $u_{\text{st},l,j} = (-1)^l (-u_{l-1,j} + 2u_{l,j} - u_{l+1,j})/4$, while the ionicity $\rho_{l,j}$ is defined as $\rho_{l,j} = 1 + (-1)^l (-\langle n_{l-1,j} \rangle + 2\langle n_{l,j} \rangle - \langle n_{l+1,j} \rangle)/4$.

![Figure 1](image1.png)

**Figure 1.** Staggered lattice displacement $u_{\text{st},l,j}$ (vertical component of each bar) and ionicity $\rho_{l,j}$ (horizontal component of each bar), as a function of the site index $(j-1)L+l$ and the dimensionless time $\omega_{\text{opt}} t$ during the oscillating electric field is applied to the ionic phase with $U_{\perp}=V_{\perp,1}=0$.

![Figure 2](image2.png)

**Figure 2.** Staggered lattice displacement $u_{\text{st},l,j}$ (vertical component of each bar) and ionicity $\rho_{l,j}$ (horizontal component of each bar), as a function of the site index $(j-1)L+l$ and the dimensionless time $\omega_{\text{opt}} t$ during the oscillating electric field is applied to the neutral phase with $U_{\perp}=V_{\perp,1}=0$.

When the regular neutral phase is photoexcited, the transition into the ionic phase takes place
in an uncooperative manner [13]. The final ionicity is almost a linear function of the increment of the total energy. Its linear coefficient is almost independent of the frequency of the electric field, and of the degree of the initial lattice fluctuations [14]. Thus the final state is determined merely by how many photons are absorbed to increase the ionicity. If the electric field is turned off during the transition, the electronic state remains intermediate between the neutral and ionic states. This is a consequence of the fact that ionic domains, if created, do not spontaneously grow (figure 2). These findings are consistent with the latest experiments [8]. In the final ionic state, the staggered lattice displacements appear, but their phases are always disordered. This situation can be modified by the interchain elastic coupling in multi-chain systems, as mentioned below.

The difference of the ionic-to-neutral and neutral-to-ionic transitions is manifested by an interference effect [15]. The pulse of oscillating electric field is split into two and their interval is varied. In the ionic-to-neutral transition, the two pulses constructively interfere with each other if the interval is a multiple of the period of the optical lattice vibration, while they destructively interfere if the interval is a half-odd integer times the period. This clear interference effect is due to the coherence of the ionicity and the dimerization. In the neutral-to-ionic transition, however, the interference effect is very weakly observed because the photoinduced lattice oscillations have random phases.

2.2. Effects of interchain couplings

For simplicity, we first consider the case with $t_0=\beta_2=0$ and ignore the edge chains. The total energy per donor-acceptor unit is $E_N = -d + U$ in the neutral phase, and $E_I = -2V + 2U_\perp - 2V_{\perp 1} - 2V_{\perp 2}$ in the ionic phase. The energy difference is then given by $E_N - E_I = U + 2V - d_{\text{ren}}$, where $d_{\text{ren}} = d + 2U_\perp - 2V_{\perp 1} - 2V_{\perp 2}$. In the calculations, we use $d_{\text{ren}}=2.716\text{eV}$ to make the two phases have nearly equal energies.

The intramolecular charge distribution in each constituent molecule is calculated by the ab initio quantum chemical method [16]. The electrostatic energies between neighboring molecules are estimated as $V=1.26\text{eV}$, $U_\perp=0.94\text{eV}$, and $V_{\perp 1}=1.08\text{eV}$. Because the molecules are tilted, the relative repulsion strengths are quite different from the naive expectations based on the intramolecular distance measured in terms of the center of mass of each molecule. Thus $V_{\perp 2}$ is much smaller than $V_{\perp 1}$. In these estimations, the kinetic energy of itinerant electrons hopping among neighboring molecules is not taken into account. Then these values would give upper bounds for the repulsion strengths. Simply by adopting the ratios $U_\perp/V$ and $V_{\perp 1}/V$ and the value $V=0.604\text{eV}$ [10], we roughly obtain $U_\perp=0.45\text{eV}$ and $V_{\perp 1}=0.50\text{eV}$. We calculated with $U_\perp/V_{\perp 1}=0.9$ and $V_{\perp 2}=0$ to find smooth changes from the results at $V_{\perp 1}=0$ to those at $V_{\perp 1}=0.50\text{eV}$.

The pressure-temperature phase diagram of the TTF-CA complex [17] is reproduced in the anisotropic Blume-Emery-Griffiths model, where the pseudo-spin variables $0$ and $\pm 1$ are assigned to the neutral state and the two ionic states with different polarizations [18]. The domain wall energy $E_{\text{DW}}=450\text{K}$, the interchain non-polar coupling strength $K_\perp=90\text{K}$, and the interchain polar coupling strength $J_\perp=5\text{K}$ are used to reproduce the triple point at $220\text{K}$, the critical temperature on the condensation line at $260\text{K}$, and discontinuous melting. In order to reproduce the slope of the condensation line, the interchain electrostriction needs to be taken into account [19]. In any case, the relation $J_\perp \ll K_\perp$ holds. In the present model, the domain wall energy is about $E_{\text{DW}}=0.3\text{eV}$ for $U_\perp=V_{\perp 1}=V_{\perp 2}=0$ [10]. The ratio $J_\perp/E_{\text{DW}}=1/90$ and this $E_{\text{DW}}$ value give $J_\perp=0.0033\text{eV}$, which roughly corresponds to $k_{\perp 1}=2\text{eV}$ reasonably less than $k_1=4.86\text{eV}$. We calculated with different $k_{\perp 1}$ to find smooth changes from the results at $k_{\perp 1}=0$ to those at $k_{\perp 1}=2.5\text{eV}$.

In the simplest case with $t_0=\beta_2=0$ but finite interchain electron-electron interactions, the domain wall energy at $E_N=E_I$ is given by $E_{\text{DW}} = V/2 - 2U_\perp + 2V_{\perp 1} + 2V_{\perp 2}$. The optical
gap is given by \( E_{\text{opt}}^N = d_{\text{ren}} - U - V - 2U_{\perp} + 2V_{\perp 1} + 2V_{\perp 2} \) in the neutral phase, and by
\[
E_{\text{opt}}^I = -d_{\text{ren}} + U + 3V - 2U_{\perp} + 2V_{\perp 1} + 2V_{\perp 2}
\]
in the ionic phase. Because of the relation \( U_{\perp} \sim V_{\perp 1} \gg V_{\perp 2} \), the domain wall energy and the optical gaps are not drastically modified by the interchain electron-electron interactions. Note that the magnitudes of the optical gaps are used to derive the model parameters [10]. It is fortunate that the model parameters need not be reconsidered except for \( d \). We first study the effects of the interchain electron-electron interactions by setting \( U_{\perp}/V_{\perp 1} = 0.9 \) and \( V_{\perp 2} = k_{\perp 1} = 0 \).

When the dimerized ionic phase is excited by a sufficiently high density of photons, the transition toward the regular neutral phase proceeds again in a highly cooperative manner. If the absorption of photons is not sufficient, the transition may be terminated with coexisting neutral and ionic chains at least on short time scales and for almost degenerate neutral and ionic phases studied here. For reasonable magnitudes of interchain electron-electron interactions, precursors of neutral domains are created but their growth is initially suppressed by the neighboring ionic domains (figure 3). When a precursor domain is first created in a chain, it increases the probability of nucleation of other neutral domains near the first one in the neighboring chains. The motions of thus created neutral domains are correlated. Then a sufficiently high density of neutral domains appear and grow together to trigger the transition.

![Figure 3](image1.png)  
**Figure 3.** Staggered lattice displacement \( u_{\text{st}, l,j} \) (vertical component of each bar) and ionicity \( \rho_{l,j} \) (horizontal component of each bar), as a function of the site index \(( j-1)L + l \) and the dimensionless time \( \omega_{\text{opt}} t \) during the oscillating electric field is applied to the ionic phase with \( U_{\perp} = 0.36 \) and \( V_{\perp 1} = 0.40 \).

![Figure 4](image2.png)  
**Figure 4.** Staggered lattice displacement \( u_{\text{st}, l,j} \) (vertical component of each bar) and ionicity \( \rho_{l,j} \) (horizontal component of each bar), as a function of the site index \(( j-1)L + l \) and the dimensionless time \( \omega_{\text{opt}} t \) during the oscillating electric field is applied to the neutral phase with \( U_{\perp} = 0.36 \) and \( V_{\perp 1} = 0.40 \).

When the regular neutral phase is photoexcited, the transition toward the ionic phase proceeds again in an uncooperative manner. After the electric field is turned off, the ionicity does not significantly change even if the transition is not completed. The final ionicity is almost a linear function of the increment of the total energy. Its linear coefficient is almost independent of the interchain electron-electron interactions as long as the relation \( U_{\perp} \sim V_{\perp 1} \gg V_{\perp 2} \) is satisfied. Interchain electron-electron interactions may promote creation of locally ionic domains (figure 4), but such ionic domains do not grow without energy supply from the oscillating electric field.

The interchain electron-electron interactions significantly slow down both the ionic-to-neutral transition (compare figures 1 and 3) and the neutral-to-ionic transition (compare figures 2 and 4). In the ionic-to-neutral transition, the threshold absorption increases with the interchain electron-electron interactions. In the present 10-chain systems, the threshold value for \( U_{\perp} = 0.45 \) eV and
$V_{11}=0.50$eV is roughly twice as much as that without interchain couplings, although the time required for the transition to be completed becomes significantly large.

In the neutral-to-ionic transition, interchain elastic couplings would be important in forming a dimerization-induce ferroelectric order. Then the effect of the $k_{1\perp}$ term is studied by setting $U_1=V_{11}=V_{22}=0$ for simplicity. We have not so far found a numerical solution where the ferroelectric order is formed. If a sufficiently large electron-lattice coupling that modulates the transfer integral [20, 21] is included furthermore, a long-range ferroelectric order is found to be formed. In such a case, the optical phonon is significantly softened in the neutral phase, enhancing the dielectric fluctuations. It contradicts the optical phonon frequency experimentally observed in the neutral phase. Electron correlations may be necessary to achieve a transition into the ferroelectric ionic phase.

3. Characteristics of field-effect transistors

In order to study the current-voltage characteristics in metal-insulator-semiconductor field-effect transistor device structures based on organic single crystals of quasi-one-dimensional insulators, we add a scalar potential $v_l$ to the one-dimensional Hubbard model for insulators, to which the tight-binding model is attached for metallic electrodes,

$$H = \sum_l (\epsilon_l + v_l) n_l - \sum_{l,\sigma} \left[ t_{l,l+1} c_{l,\sigma}^\dagger c_{l+1,\sigma} + t_{l+1,l} c_{l+1,\sigma}^\dagger c_{l,\sigma} \right] + \sum_l U_l \left( n_l^\uparrow - \frac{1}{2} \right) \left( n_l^\downarrow - \frac{1}{2} \right),$$

where the site energy $\epsilon_l$ is set at $-\phi$ in the crystal and at 0 in the electrodes. The absolute value of the transfer integral $|t_{l,l+1}|$ is set at $t_c$ if either $l$ or $l+1$ is in the crystal and at $t_e$ otherwise. The on-site repulsion $U_l$ is set at $U$ in the crystal and at 0 in the electrodes. When we consider band insulators, we use $U=0$ and replace $t_c$ by $t_c - (1/\beta t)$. The periodic boundary condition is imposed by introducing the Peierls phase to the transfer integral for finite drain voltage $V_D$.

The scalar potential $v_l$ obeys the Poisson equation on the discrete lattice,

$$v_{l+1} - 2v_l + v_{l-1} = -V_{PI} (\langle n_l \rangle - n_{BL}) ,$$

where the parameter $V_{PI}$ comes from the long-range Coulomb interaction and $n_{BL}$ from the background charge. The parameter $V_{PI}$ is set at $V_{Pc}$ in the crystal and at $V_{Pe}$ in the electrodes, with $V_{Pe} \ll V_{Pc}$. The gate bias $U_G$ defined in [9] is assumed to appear with the gate efficiency factor $\alpha$ in the boundary value of the Poisson equation,

$$v_{L/2} - v_0 = -\alpha U_G + \phi ,$$

where $l = L/2$ is set at the middle of the crystal and $l = 0$ in the electrode is the furthest point from the crystal-electrode interfaces. Hereafter we rewrite $\alpha U_G$ as $U_G$ for simplicity.

We numerically solve the time-dependent Schrödinger equation in the unrestricted HF approximation simultaneously with the Poisson equation. The self-consistency is imposed at each time and site in these equations. The drain current $I_D$ is obtained in the same manner as in [22], by averaging the current density over the period $0 < t < \Delta t$ with $\Delta t = 2\pi L/(4V_D)$. For calculations, we use $t_e=1$, as a unit, and $U=2$ for Mott insulators, which produces a charge gap of about $\Delta CG=0.68$ at half filling in the present approximation. We use $t_e=1$ simply because the numerical convergence is generally stable and rapid for comparable transfer integrals, but the main conclusion is not altered by different transfer integrals. We use $V_{Pe}=0.05$ and $V_{Pc}=10^{-3}$, but the main conclusion is again not altered by different Coulomb parameters. Periodic systems with $L=100$ sites are used, in which 51 sites belong to the crystal and 49 sites to the electrodes.
3.1. Difference of Mott and band insulators

Mott insulators show nearly symmetric $I_D-U_G$ characteristics even for finite work-function differences (figure 5). For small $V_D$ and $| U_G |$ that is smaller than a half of the charge gap, $I_D$ is suppressed. The drain current $I_D$ increases with electron injections ($U_G > 0$) and with hole injections ($U_G < 0$) in a similar manner. For the gate-bias polarity with higher Schottky barriers ($U_G > 0$ in the present case), the correlation effect is weakened. This balancing of the correlation effect with the barrier effect causes the ambipolar characteristics. In the calculation, the work function of the metallic electrodes is higher than that of the crystal by $-\phi=1.0$.

![Figure 5](image) ![Figure 6](image)

**Figure 5.** $I_D-U_G$ characteristics at various $V_D$ for Mott insulators with $U=2$.

**Figure 6.** $I_D-U_G$ characteristics at various $V_D$ for band insulators with $\delta t=0.17$.

For band insulators, we use $\delta t=0.17$, which also gives a charge gap of $\Delta_{CG}=0.68$ at half filling. Band insulators clearly show very asymmetric $I_D-U_G$ characteristics for finite work-function differences (figure 6). The Schottky barriers with $\phi < 0$ are higher for the electron injections $U_G > 0$ than for the hole injections $U_G < 0$ at a given $| U_G |$. The drain current $I_D$ increases with the hole injections, but it remains suppressed for the electron injections. These unipolar field-effect characteristics in band insulators are generally obtained irrespective of whether the charge gap is introduced by alternating transfer integrals, alternating site energies, or staggered magnetic fields. They are in marked contrast to the ambipolar field-effect characteristics in Mott insulators, where the charge gap is introduced by the electron-electron interaction.

4. Summary

We have shown two examples where electron-electron interactions are crucial to determine the nonequilibrium properties of low-dimensional electron systems. First, in a quasi-one-dimensional extended Peierls Hubbard model with alternating potentials for the TTF-CA complex, the photoinduced ionic-to-neutral transition is shown to be different from the photoinduced neutral-to-ionic transition. The former is characterized by the threshold intensity of photoexcitation. This is due to spontaneous and cooperative growth of metastable neutral domains after they overcome the initial competition with stable ionic domains in neighboring chains. Because the nonlinearity or linearity in the final ionicity as a function of the supplied energy is maintained even if the electron-lattice coupling is switched off, whether the initial state is either a Mott insulator or a band insulator appears important. Second, in a one-dimensional Hubbard model with scalar potentials for Schottky barriers at interfaces with metallic electrodes, the field-effect characteristics are shown to be ambipolar for Mott insulators, while generally unipolar for band insulators due to work-function differences. The former is due to balancing of the correlation effect with the barrier effect, which is again characterized by the cooperativity of charge transport in the strongly correlated electronic background.
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