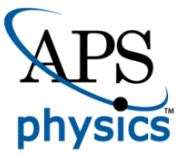

Equivalent Resistance from the Quantum to the Classical Transport Limit

Saheli Sarkar, Damaris Kröber, and Dirk K. Morr

Phys. Rev. Lett. **117**, 226601 — Published 23 November 2016

DOI: 10.1103/PhysRevLett.117.226601

Equivalent Resistance from the Quantum to the Classical Transport Limit

Saheli Sarkar, Damaris Kröber, and Dirk K. Morr*
University of Illinois at Chicago, Chicago, IL 60607, USA
(Dated: October 21, 2016)

We generalize the concept of equivalent resistance to the entire range from coherent quantum to diffusive classical transport by introducing the notion of transport equivalent networks. We show that this novel concept presents us with a platform to simplify the structure of quantum networks while preserving their global and local transport properties, even in the presence of electron-phonon or electron-electron interactions. This allows us to describe the evolution of equivalent quantum networks to equivalent classical resistor networks with increasing interaction strength.

The equivalent resistance of a network of classical resistors is one of the most fundamental concepts that is used in many fields ranging from physics to engineering. It possesses two characteristic properties: (i) an equivalent resistor leaves the transport properties of the resistor network it replaces unchanged, and (ii) it simplifies the structure of the original network [1]. With the continued miniaturization of electronic circuits [2], the exploration of transport properties at the atomic scale [3–5], and the ability to design quantum structures at the nanoscale [6–8], it has become of paramount importance to explore whether this concept can be extended not only to the crossover region between classical to quantum transport [9] but indeed to the limit of full quantum coherence. Such an extension could provide a unique venue to extend Moores law [10] into the regime of quantum transport, opening unprecedented opportunities for the creation of novel transport functionalities.

In this Letter, we demonstrate that the concept of a classical equivalent resistance can be generalized to the entire range from quantum to classical transport by introducing the concept of transport equivalent networks (TENs). To this end, we describe the electronic structure of a system in terms of a quantum network [11–13] [see Fig.1(a)] and define two networks to be transport equivalent, if they possess identical IV-curves for any applied gate voltage. For transport equivalence between networks to exist, it is a sufficient condition that the networks' Hamiltonians are connected by a unitary transformation. This satisfies requirement (i) of an equivalent resistor. To address requirement (ii) – the simplification of a network – we note that in a network such as the one shown in Fig.1(a), there exist electronic states that do not take part in charge transport since they possess zero spectral weight at the sites that are connected to the leads. Such states can therefore be eliminated from the network, leading to a simpler structure, without modifying its transport properties. We will show that transport equivalence holds even in the presence of electron-phonon or electron-electron interactions, allowing us tune networks from the non-interacting quantum to the classical transport regime while maintaining their transport equivalence. This enables a mapping of transport equivalent quantum networks onto transport equivalent classical resistor networks, and generalizes the concept of an equivalent resistor to the entire regime from quantum to classical transport.

To generalize the concept of an equivalent resistor, we represent the electronic structure of a system as a network [11–15] of connected sites that is attached to two (or more) leads, as shown in Fig.1(a), described by the Hamiltonian $H = H_0 + H_{ee} + H_{ph} + H_{lead}$ where

$$H_0 = \sum_{i,j,\sigma} \left(-t_{ij} - E_0\delta_{ij}\right) c^\dagger_{i,\sigma} c_{j,\sigma} - t_l \sum_{\mathrm{r},i,\sigma} \left(d^\dagger_{\mathrm{r},\sigma} c_{i,\sigma} + h.c.\right) \ . \tag{1}$$

Here $-t_{ij}$ and E_0 are the hopping amplitude between sites i and j in the network, and the local on-site energy, respectively, and $c^\dagger_{i,\sigma}$ ($d^\dagger_{i,\sigma}$) creates a fermion with spin σ at site i in the network (leads). The second term describes the coupling of the network to M leads with hopping amplitude $-t_l$. Moreover, H_{ee} and H_{ph} describe the electron-electron and electron-phonon interactions in the system (to be discussed below) and H_{lead} represents the electronic structure of the leads. For the subsequent discussion, it is beneficial to rewrite H_0 in matrix form as $H_0 = \sum_\sigma \Psi^\dagger_\sigma \hat{H}_0 \Psi_\sigma$ with $\Psi^\dagger_\sigma = \left(d^\dagger_{1\sigma}, \ldots, d^\dagger_{M\sigma}, c^\dagger_{1\sigma}, \ldots, c^\dagger_{N\sigma}\right)$ being a spinor with the indices of its elements running over all sites in the leads and network, and $\hat{H}_0$ being the Hamiltonian matrix. To compute the charge transport in such networks, we employ the non-equilibrium Keldysh Green's function formalism [16–18] where the charge current between sites i and j in the network is given by

$$I_{ij} = -2g_s \frac{e}{\hbar} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left(-t_{ij}\right) Re\left[G^<_{ij}(\omega)\right] , \tag{2}$$

with $G^<_{ij}(\omega)$ being the full lesser Green's function (see supplemental information (SI) Sec. I), and $g_s = 2$ representing the spin degeneracy. A current is induced by applying different chemical potentials, $\mu_{L,R} = \pm e\Delta V/2$ in the left (L) and right (R) leads, resulting in a voltage bias ΔV across the network.

A sufficient condition for two networks to be transport equivalent is that their respective Hamiltonian matrices, $\hat{H}_0$ and $\hat{H}'_0$ are related by a unitary transformation $\hat{U}$,

i.e., $\hat{H} = \hat{U}\hat{H}_0\hat{U}^\dagger$ (see SI Sec. II). This equivalence holds irrespective of the specific form of H_{lead}. Additionally, we require that the electronic and spatial coupling to the leads be the same for both networks, implying that the M sites, through which the current enters or exits the networks as well as the M lead sites, are unaffected by the unitary transformation. As a result, $\hat{U}$ possesses the following matrix representation

$$\hat{U} = \begin{pmatrix} \hat{1} & \hat{0} \\ \hat{0} & \hat{Q} \end{pmatrix} \tag{3}$$

where $\hat{1}$ is the $2M \times 2M$ identity matrix that acts on the M network sites and the M leads that are connected, and $\hat{Q}$ is an $(N-M) \times (N-M)$ unitary matrix that acts on all other sites of the network.

To exemplify the concept of transport equivalent networks, we consider a network with two parallel branches [Fig. 1(a)] which represents the quantum analog of a classical parallel resistor network. Using the numbering of sites shown in Fig. 1(a), the unitary transformation

$$\hat{U} = \begin{pmatrix} \hat{1} & 0 & 0 \\ 0 & \hat{D}(\alpha) & 0 \\ 0 & 0 & \hat{D}(\beta) \end{pmatrix} \tag{4}$$

where $\hat{D}(\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}$ yields a whole class of TENs whose electronic hopping elements are parameterized by the angles α and β [see Fig. 1(b)]. While all of these TENs possess identical transport properties, they are in general, however, not simpler than the original network since even new hopping elements can emerge. The main challenge therefore lies in finding a transformation $\hat{U}$ that yields the largest possible simplification of a network, with the exact meaning of simplification being dependent on the particular network properties one might be interested in. For example, the network of Fig. 1(b) can be simplified to a smaller network by choosing $\alpha = \beta = \pi/4$ [Fig. 1(c)]. In this case the TEN separates into two disjoint parts, of which only one is connected to the leads and thus contributes to charge transport. The disconnected part can therefore be omitted, implying that the original network [Fig. 1(a)] consisting of six sites can be replaced by a simpler (i.e., smaller) network with identical transport properties that consists of four sites with renormalized hopping amplitudes [Fig. 1(c)]. The IV curves of the original network [Fig. 1(a)] and of the TEN [Fig. 1(c)] computed from Eq.(2) are as expected identical [see Fig. 1(d)]. This result can immediately be generalized to a network with P parallel branches each consisting of K sites [Fig. 1(e)] with the smallest TEN possessing only a single branch [Fig. 1(f)] (the explicit form of $\hat{U}$ is given in SI Sec. III.A). Identifying the unitary transformation that yields the simplest TEN thus represents the quantum analog of finding the classical equivalent resistor.

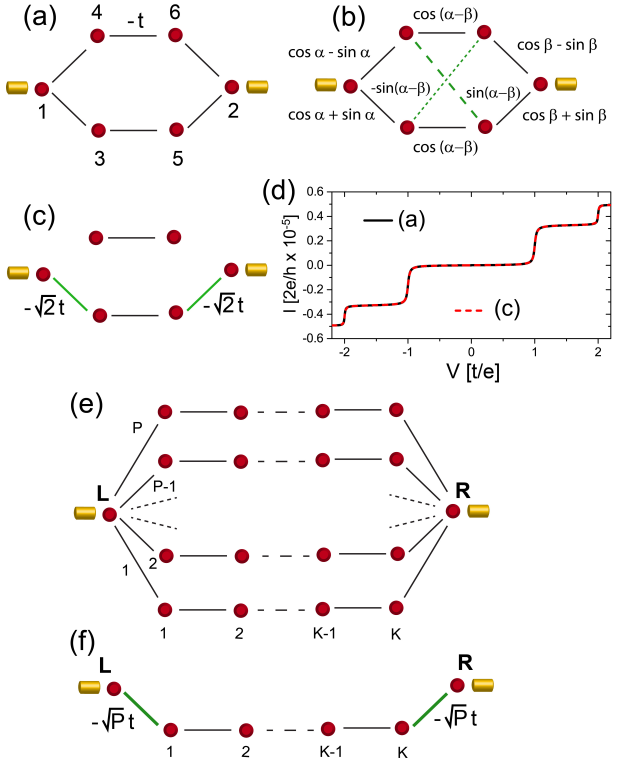

FIG. 1. (a) Quantum network with two parallel branches (black lines represent a hopping $-t$). (b) TEN to (a) for arbitrary α, β (hopping elements are given in units of $-t$).(c) Simplest transport equivalent network to (a) for $\alpha = \beta = \pi/4$. (d) IV-curves for the networks in (a) and (c).(e) Multi-branch network, and (f) its simplest TEN (green lines represent a hopping of $-\sqrt{Pt}$).

The concept of transport equivalence can be applied to a wide variety of networks such as networks containing next nearest-neighbor hopping amplitudes [Figs. 2(a), (b), the corresponding $\hat{U}$ is given in SI Sec. III.B], networks with a square lattice or graphene lattice structure (see SI Sec. III.C), networks that include disorder in the on-site energies or hopping amplitudes [Figs. 2(c), (d), see SI Sec. III.D], or three-dimensional networks [Figs. 2(e) - (h), SI Sec. III.E]. All of the TENs shown in the right column of Fig. 2 are TENs with the smallest number of network sites and hopping elements, thus realizing the greatest simplification of the original networks (left column). The number of networks sites in the smallest possible TEN can be deduced from the original network: if the original network of N sites possesses N_0 states whose wave-functions simultaneously vanish at all sites that the leads are connected to, then this network can be transformed into a class of smallest TENs in which only $S_{min} = N - N_0$ sites are connected to the leads, while the remaining N_0 sites are disconnected and therefore irrelevant for charge transport. For example, the network shown in Fig. 1(e) possesses $(P \times K + 2)$ sites and $(P-1) \times K$ states whose wave-function van-

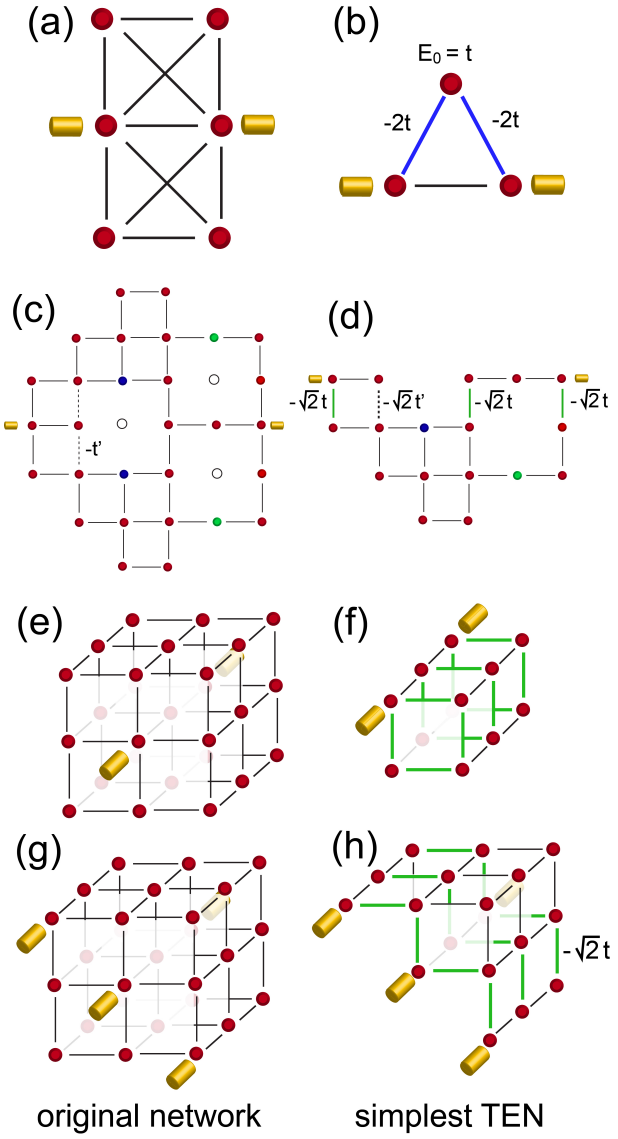

FIG. 2. (a) Network with next-nearest neighbor hopping, and (b) its simplest TEN (unless otherwise noted, $E_0 = 0$). (c) Disordered network (open circles represent missing sites, circles of the same color possess the same E_0, dotted line represents a hopping of $-t'$), and (d) its simplest TEN. Three-dimensional networks with different leads possessing (e) a C_4, and (g) a C_2 symmetry around their center axis. (f),(h) Simplest TENs to (e) and (g). Blue and green lines represent hoppings of $-2t$ and $-\sqrt{2}t$, respectively.

ishes at sites **L** and **R** which are connected to the leads. It can therefore be transformed into a new network with $S_{min} = K + 2$ sites [Fig. 1(f)] that does not only contain the smallest of possible number of sites, but also of hopping elements, and therefore represents the simplest possible TEN. We note that systems (i.e., network and leads) that have a higher symmetry [such as that in Fig. 2(e) with C_4-symmetry] in general possess TENs with a smaller S_{min} than systems with a lower symmetry [such as that in Fig. 2(g) with C_2-symmetry].

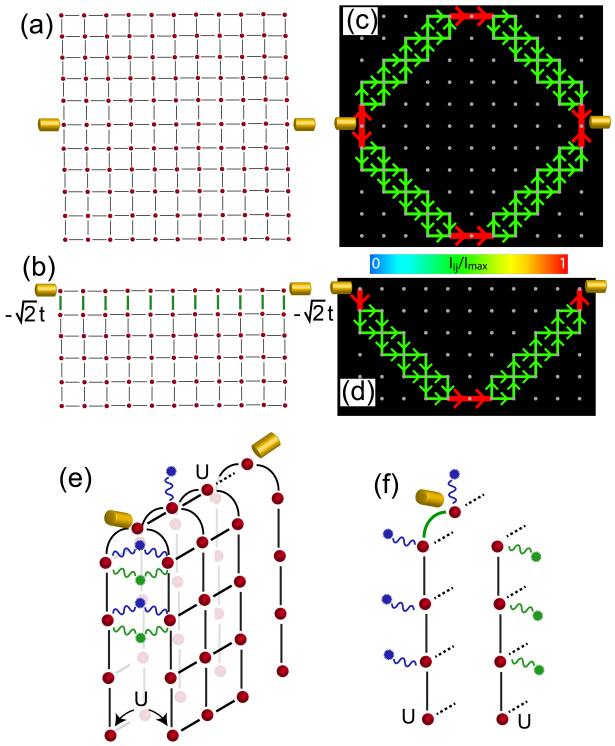

FIG. 3. (a) Square-lattice network, and (b) its simplest TEN. (c),(d) Spatial pattern of the normalized currents carried by the $E = 0$ state in the networks of (a) and (b) for $\Delta V = 0.01t/e$. (e) "Bent" square lattice network with sites symmetric around the center row interacting with the same two phonon modes (blue and green wavy line) and via an electron-electron interaction U. (f) Simplest TEN to (e).

The transport equivalence of networks is also reflected in a close similarity of their spatial current patterns. To demonstrate this, we consider the $N_x \times N_y$ square lattice network shown in Fig. 3(a) (with $N_x = N_y = 11$), and its smallest TEN consisting of $N_x(N_y+1)/2$ sites [Fig. 3(b), see SI Sec. III.C]. In this TEN, only the vertical hopping elements directly connected to the top row are modified to $-\sqrt{2t}$ in comparison to the original network. The IV curves of these two networks are identical (see SI Sec. IV), and the spatial patterns of current flow through both networks [see Figs. 3(c) and (d)] exhibit a close similarity, in that the current pattern in the TEN is all but identical to that in the lower half of the original network. This similarity also holds for the current patterns carried by other energy states and in networks with $N_x \neq N_y$ (see SI Sec. IV), and thus establishes the equivalence of not only global but also local transport properties.

The concept of transport equivalent networks can also be extended to interacting networks containing electron-electron or electron-phonon interactions. In this case, a simpler TEN exists if the form of the interactions in the original network is such that after applying the unitary

transformation, the interaction does not couple the disjoint parts in the TEN. To demonstrate this, we consider a bent square-lattice network [Fig. 3(e)] in which electrons on sites i and j (which are symmetric with respect to the center row) interact with the same two phonon modes as described by

$$H_{ph} = \frac{g}{2}\sum_{\langle i,j\rangle,\sigma}\Big[(n_{i,\sigma}+n_{j,\sigma})\left(a_i^\dagger + a_i + a_j^\dagger + a_j\right) + \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}\right)\left(a_i^\dagger + a_i\ - a_j^\dagger - a_j\right)\Big] + g\sum_{r,\sigma} n_{r,\sigma}\left(a_r^\dagger + a_r\right) + \sum_k \omega_k a_k^\dagger a_k\ . \quad (5)$$

Here, $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ is the local occupation operator, g is the interaction strength, and the first sum runs over all pairs of symmetric pairs of sites i and j, the second sum runs over the sites of the middle row, and the last one over all phonon modes with energy ω_k. In the TEN [Fig. 3(f), using the unitary transformation of Eq.(S32) in SI Sec. IIIC], the electron-phonon interaction is entirely local and given by

$$H_{ph}^{'} = g\sum_{i,\sigma}\left(a_i^\dagger + a_i\right) + \sum_k \omega_k a_k^\dagger a_k\ . \quad (6)$$

Thus, the unitary transformation yields two disjoint parts of the TEN, even in the presence of the electron-phonon interactions and we can again neglect the part disconnected from the leads. Similarly, an electron-electron interaction in the original network of the form [Fig. 3(e)]

$$H_{ee} = \frac{U}{2}\sum_{\langle i,j\rangle}(c_{i\uparrow}^\dagger c_{j\uparrow} c_{i\downarrow}^\dagger c_{j\downarrow} + c_{i\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{i\downarrow}) + \frac{U}{2}\sum_{\alpha,\beta=\langle i,j\rangle} n_{\alpha\uparrow}n_{\beta\downarrow} + U\sum_r n_{r\uparrow}n_{r\downarrow} \quad (7)$$

transforms into a purely local Coulomb interaction in the TEN [Fig. 3(f)]

$$H_{el} = U\sum_i n_{i\uparrow}n_{i\downarrow} \quad (8)$$

allowing us to again neglect the disjoint part of the TEN.

To demonstrate the transport equivalence of networks in the presence of an electron-phonon interaction, we consider the Hamiltonians of Eqs.(5) and (6) in the networks of Figs. 3(a) and (b), respectively. The computational evaluation of their transport properties is in general quite demanding for arbitrary temperature and phonon energy ω_k. We therefore simplify this task by considering a single phonon energy $\omega_k = \omega_0$ in the high-temperature limit $k_BT \gg \hbar\omega_0$ [19] (see SI Sec. I) yielding an effective electron-phonon interaction given by $\zeta = 2g^2k_BT/(\hbar\omega_0)$. Not only is the resulting total current through these networks identical for all ζ [Fig. 4(a)], but the close similarity of the spatial current patterns in the TENs also

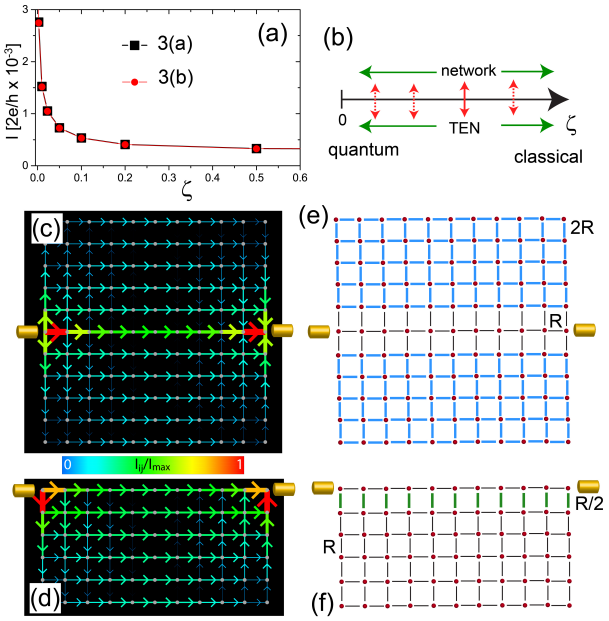

FIG. 4. (a) Current through the networks of Fig. 3(a) and (b) as a function of ζ for $\mu_{L,R} = \pm 0.005t$. (b) Schematic representation of the transport equivalence between networks holding over the entire range of ζ from the quantum to the classical transport regime. (c),(d) Spatial pattern of the normalized current carried by the $E = 0$ state in the networks of Figs. 3(a) and (b) for $\Delta V = 0.0004t/e$ and $\zeta = 50t^2$, approaching the classical limit $\zeta \to \infty$. (e),(f) Classical resistor networks that possess the same spatial current patterns as in (c) and (d). Black, blue and green lines represent a resistance of R, $2R$, and $R/2$, respectively.

persists over the entire range from the quantum $\zeta = 0$ [Figs. 3(c) and (d)] to the classical $\zeta \to \infty$ transport limit [9] [Figs. 4(c) and (d), SI Sec. V]. In the latter limit, the TENs' current patterns are identical to those of the (equivalent) classical resistor networks [1] shown in Figs. 4(e) and (f) (SI Sec. VI). Thus, the networks' transport equivalence holds for all strengths of the electron-phonon interaction, as schematically shown in Fig. 4(b), demonstrating that the concept of transport equivalent networks can be extended to the entire range from quantum to classical transport.

We note that the above generalization of the equivalent resistance should be applicable to any system in which transport can be described within the above formalism, such as networks of quantum dots [20, 21], molecules and polymers [22], and excitonic energy transfer networks in lightharvesting complexes [14, 23, 24]. Moreover, it will allow us to create and identify networks with very different local electronic structures, and hence local current patterns, which are nevertheless transport equivalent [25]. This clearly establishes the wide-ranging importance and appeal of this novel concept in exploring and discovering transport phenomena in a broad range of materials and systems. Finally, an interesting exten-

sion of the above work is to relax the requirement of exact transport equivalence, and to consider networks that are "nearly" transport equivalent. We expect that this would allow us to further reduce the size of networks, and to consider simpler forms of interactions.

We would like to thank T. Can, D. Goldhaber-Gordon, and M. Vojta for helpful discussions. This project was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-FG02-05ER46225.

* dkmorr@uic.edu

[1] F. Y. Wu, J. Phys. A-Math. Gen. **37**, 6653 (2004).
[2] W. Lu and C. M. Lieber , Nat. Mater. **6**, 841 (2007).
[3] B. Weber *et al.*, Science **335**, 64 (2012).
[4] M. Fuechsle *et al.*, Nat. Nanotechnolo. **7**, 242 (2012).
[5] F. A. Zwanenburg *et al.*, Rev. Mod. Phys. **85**, 961 (2013).
[6] K. K. Gomes, W. Mar, W. Ko, F. Guinea, and H. C. Manoharan, Nature **483**, 306 (2012).
[7] A. Singha *et al.*, Science **332**, 1176 (2011).
[8] M. A. Topinka *et al.*, Science **289**, 2323 (2000).
[9] D. K. Morr, Contemp. Phys. **57**, 19 (2016).
[10] G. E. Moore, Proceedings of the IEEE **86**, 82 (1998).
[11] A. Cresti, R. Farchioni, G. Grosso, and G. P. Parravicini, Phys. Rev. B **68**, 8 (2003).
[12] T. N. Todorov, J. Phys-Condens. Mat. **14**, 3049 (2002).
[13] T. N. Todorov, Philos. Mag. B **79**, 1577 (1999).
[14] K. M. Pelzer, T. Can, S. K. Gray, D. K. Morr, and G. S. Engel, J. Phy. Chem. B **118**, 2693 (2014).
[15] J. Figgins, and D. K. Morr, Phys. Rev. Lett. **104**, 4 (2010).
[16] L. V. Keldysh, Sov. Phys. Jetp-Ussr **20**, 1018 (1965).
[17] C. Caroli, R. Combesco, P. Nozieres, and D. Saintjam, J. Phys. C Solid State **4**, 916 (1971).
[18] J. Rammer, and H. Smith, Rev. Mod. Phys. **58**, 323 (1986).
[19] Z. Bihary, and M. A. Ratner, Phys. Rev. B **72**, 115432 (2005).
[20] D. V. Talapin, J. S. Lee, M. V. Kovalenko, and E. V. Shevchenko, Chem. Rev. **110**, 389 (2010).
[21] R. Parthasarathy, X. M. Lin and H. M. Jaeger, Phys. Rev. Lett. **87**, 4 (2001).
[22] B. Moulton, and M. J. Zaworotko, Chem. Rev. **101**, 1629 (2001).
[23] G. D. Scholes, and G. Rumbles, Nat. Mater. **5**, 683 (2006).
[24] G. D. Scholes, G. R. Fleming, A. Olaya-Castro, and R. van Grondelle, Nat. Chem. **3**, 763 (2011).
[25] S. Sarkar and D.K. Morr, unpublished.