PHYSICAL REVIEW A **109**, L060801 (2024)

Letter

Charge transfer via temporary bonds in $C_{60} + C_{60}{}^{+}$ molecular collisions

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(Received 21 July 2023; revised 8 January 2024; accepted 29 February 2024; published 3 June 2024)

We present a theoretical description of resonant charge transfer in collisions of nanoparticles, specifically for $C_{60} + C_{60}{}^{+}$ collisions. We predict that transient bonds between colliding fullerenes can significantly extend the interaction time, allowing for a greater probability of charge transfer. In our model, the dumbbell-shaped $(C_{60} - C_{60})^{+}$ quasimolecule, that is temporarily formed during the collision, is described as a dynamic system of 120 zero-range potentials. Using this model, we calculate the exchange interaction between colliding fullerenes and subsequently determine the corresponding charge-transfer cross sections at different collision velocities. Our results have been verified with data obtained from quantum molecular dynamics simulations of the fullerene collisions. The presented theoretical model provides a description of the experimental data on the $C_{60} + C_{60}{}^{+}$ resonant charge-transfer collision through the inclusion of the temporary formation of dumbbell-shaped fullerene molecules at low collision velocities.

DOI: 10.1103/PhysRevA.109.L060801

Introduction. Investigations of charge-transfer processes have a rich history due to many applications in plasma physics, astrophysics, atmospheric science, and chemistry [1–3]. In atom-ion systems, the physics of charge-transfer collisions is well understood and the probabilities of the underlying quantum processes can be determined with high-accuracy *ab initio* calculations [4–6]. A significantly higher level of complexity arises in molecular charge-transfer processes because the dynamics of the nuclear degrees of freedom may strongly influence the parameters of the exchange interaction between colliding particles. Since the advent of ultrafast laser pulses, charge-transfer collisions have also been used to probe fundamental quantum dynamics as these reactions are heavily dependent on the properties of the electronic wave function [7]. Recently, charge-transfer research has expanded to more complex systems such as large molecules, nanosize clusters, and condensed matter materials [8–11]. Fullerenes have become a popular molecule to study due to their high degree of symmetry [12] and potential technological applications [9,13,14].

Total cross sections for $C_{60} + C_{60}{}^{+}$ resonant charge-transfer collisions were first measured by Rohmund and Campbell in 1997 [15]. Their experiment was arranged to detect charge transfer for small scattering angles only because of numerous studies of ions colliding with atoms or molecules. Glotov and Campbell later discovered C_{60} resonant charge transfer at large scattering angles and used these results to update the originally published total cross-section data [16].

Several models [17–19] have been employed to explain the results of the small scattering angle measurements [15]. Charge transfer at large scattering angles implies that a noticeable portion of the charge-transfer cross section is due to collisions where the C_{60} molecules overlap. These kinds of reactions were not accounted for in any of the theories describing the small scattering angle cross section. Such overlap leads to the temporary formation of the dumbbell-shaped $(C_{60} - C_{60})^{+}$ quasimolecule, with chemical bonds between atoms from different C_{60} molecules. These temporary bonds can act as "bridges," creating efficient pathways for the charge to transfer between fullerenes. These bonds are also important for the transfer of the translational kinetic energy of the fullerenes into internal degrees of freedom. These processes bring complexity into developing a consistent theoretical model but they add the possibility of using measurements of charge-transfer processes to probe the collision dynamics of the internal structure of nanoparticles. The formation of stable fullerene dimers has been investigated in several articles [20–22]. We argue that the temporary formation of dumbbell-shaped fullerene molecules can create long-lived compound states which increase the probability of charge transfer. The formation of the long-lived dumbbell-shaped $(C_{60} - C_{60})^{+}$ molecules with different orientations have been confirmed in our quantum molecular dynamics (QMD) simulations of slow fullerene collisions as well. However, realistic simulations of colliding fullerenes require the inclusion of a large number of

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excited states. This means meaningful *ab initio* calculations of collision trajectories are extremely difficult. Our QMD simulations only include the ground state, and were only meant to support our semiempirical model by demonstrating the transfer of translational kinetic energy into internal degrees of freedom.

To illustrate the impact of bridge formation on the charge-transfer cross section in $C_{60} + {C_{60}}^{+}$ collisions, we employed a simplified model of the electronic structure of C_{60} molecules. Sixty zero-range electronic pseudopotentials have been arranged in the geometry corresponding to the structure of C_{60}. The electronic energies, the wave functions, and the exchange interaction between C_{60} and ${C_{60}}^{+}$ have been calculated by combining these zero-range potential (ZRP) results with the Holstein-Herring method [23]. We computed the cross section of the charge-transfer collisions $\sigma(v)$ as a function of the collision velocity v and compared our results to experimental data. From the analysis of the experimental data, we predicted the lifetime $\tau(v)$ of the $(C_{60} - C_{60})^{+}$ quasimolecule created by the temporary chemical bonding between the C_{60} and the ${C_{60}}^{+}$.

Methods. To calculate charge-transfer cross sections we start with the definition of a cross section for semiclassical atomic and molecular collisions with a central potential,

$$\sigma = \int_0^\infty 2\pi b P(v, b) db, \tag{1}$$

where b is the impact parameter and $P(b, v)$ is the probability of charge transfer. For the resonance charge-exchange process, $P(v, b)$ can be approximated as [23]

$$P(v, b) = \sin^2 \Phi(v, b) = \sin^2 \left(\int_{-\infty}^{\infty} \frac{\epsilon_g - \epsilon_u}{2} dt \right), \tag{2}$$

where ϵ_g and ϵ_u are the energies of the gerade and ungerade states of the $C_{60} + {C_{60}}^{+}$ system. Through the use of pseudopotentials, we have developed a computationally inexpensive method for the analyses of fullerene collisions. Similar to charge-transfer processes in multielectron atom-ion collisions, we assume that during $C_{60} + {C_{60}}^{+}$ collisions there is a single active electron which is bound by $N = 120$ ZRPs with a time-dependent distance between fullerenes $R(t)$. Each fullerene is modeled as 60 ZRPs. Individual ZRPs are centered on the carbon atoms of the fullerenes and each potential corresponds to a boundary condition imposed on the wave function of the active electron $\Psi(\mathbf{r})$ at the location of the carbon atoms. This wave function is represented by a linear superposition of Green's functions [24,25] centered on the carbon atoms, $\Psi(r) = \sum_{n=1}^{N} c_i * G(\mathbf{r}, \mathbf{R}_n, \epsilon)$, where $\mathbf{R}_n$ is the radius vector of the nth carbon atom and ϵ is the energy of the active electron. In our simplest model, Green's functions can be formally expressed using the normalized wave function $\psi_n(\mathbf{r})$ of an electron bound with energy ϵ by a single ZRP,

$$\psi_n = \sqrt{2\pi\kappa}\, G(\mathbf{r}, \mathbf{R}_n, \epsilon) = \sqrt{\frac{\kappa}{2\pi}} \frac{e^{-\kappa|\mathbf{r}-\mathbf{R}_n|}}{|\mathbf{r} - \mathbf{R}_n|}, \tag{3}$$

where $\kappa = \sqrt{2|\epsilon|}$ is related to the binding energy of the active electron in the field of a single ZRP [26]. Typically, ZRP systems are treated by solving the transcendental equation produced by the 120 boundary conditions [24]. For a system of this size, however, accurate solutions to the transcendental equation are difficult to obtain. Instead, we can estimate the eigenenergies by diagonalizing the Hamiltonian of the $C_{60} - {C_{60}}^{+}$ quasimolecule, which is represented by the symmetric 120×120 matrix,

$$H = \begin{bmatrix} \epsilon_0 & \Delta_{1,2}(R_{1,2}) & \cdots & \Delta_{1,120}(R_{1,120}) \\ \Delta_{1,2}(R_{1,2}) & \epsilon_0 & \cdots & \Delta_{2,120}(R_{2,120}) \\ \vdots & \vdots & \ddots & \vdots \\ \Delta_{1,120}(R_{1,120}) & \Delta_{2,120}(R_{2,120}) & \cdots & \epsilon_0 \end{bmatrix}, \tag{4}$$

where $\Delta_{n,m}(R_{n,m})$ describes the exchange interaction between $\psi_n(\mathbf{r})$ and $\psi_m(\mathbf{r})$. These states are localized on the nth and mth carbon atoms and $R_{n,m} = |\mathbf{R}_n - \mathbf{R}_m|$ is the distance between these atoms. As a crude estimate, the energy ϵ could be set to the negative of the ionization potential of a carbon atom. However, our approach used ϵ, and the corresponding value of κ, as a fit parameter. The parameter κ was adjusted so that the computed density distribution for the active electron in C_{60} was similar to the electron density predicted by a density-functional theory calculation. In this case, we can imagine the approximated wave function as an average of all the electrons in the C_{60} molecule or as the wave function of a single positively charged hole.

In order to calculate the exchange interaction $\Delta_{n,m}(R_{n,m})$, which describes the interaction between the m and n state, we use the Holstein-Herring method [23]. The exchange interaction between two degenerated states $\psi_n(\mathbf{r})$ and $\psi_m(\mathbf{r})$ is expressed via the probability flux of the electron wave function through the plane that is perpendicular to $\mathbf{R}_{n,m}$ and halfway between the centers m and n [23],

$$\Delta_{n,m}(R_{n,m}) = 2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_n(z = 0) \times \nabla \psi_m(z = 0) \cdot \frac{\vec{R}_{n,m}}{||\vec{R}_{n,m}||} dy\, dx, \tag{5}$$

choosing the plane that is halfway between the two potentials to be the x-y plane. When using the wave function shown in Eq. (3), Eq. (5) yields the following result: $\Delta_{n,m} = \kappa \exp[-\kappa R_{n,m}/R_{n,m}]$. Since this result is analytic, populating the matrix shown in Eq. (4), and finding its eigenvalues and eigenvectors at different distances between the fullerenes can all be done at little computational cost. Figure 1 shows the electron density of a single C_{60} molecule calculated using this method, alongside the electron density of a single C_{60} molecule calculated using density-functional theory and normalized to one electron.

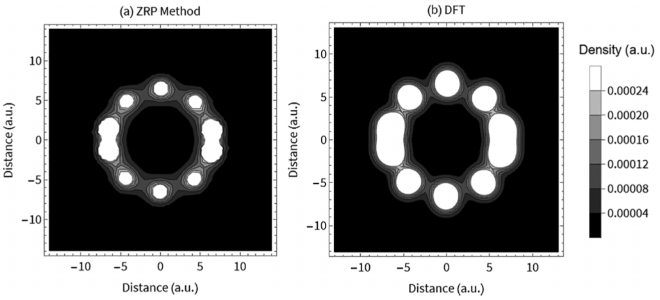

FIG. 1. The electron wave function found using the zero-range potential method (a) alongside the electron density (normalized to one) calculated using density-functional theory (b) for one plane. The zero-range potential method used κ as a fit parameter and $\kappa = 0.85$ hartree$^{1/2}$. The spots of high probability correspond to carbon nuclei. The four spots closest to the x axis are brightest since those carbon nuclei are the closest to the plane that is being plotted.

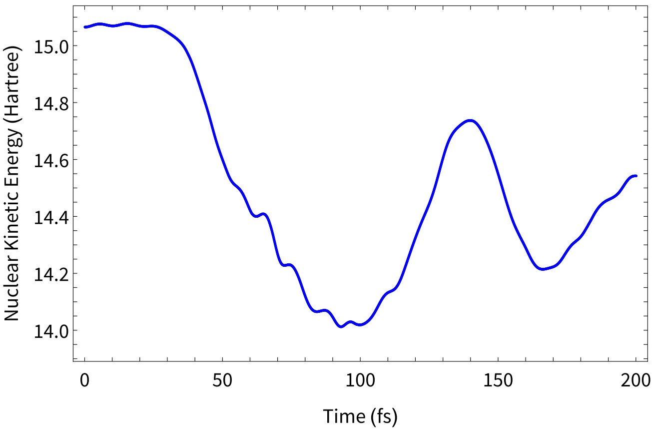

FIG. 2. The total nuclear kinetic energy as a function of time for one of our simulations. This simulation had an impact parameter of $b = 14.17a_0$ and a collision energy of 410 eV.

Computation of the charge-transfer cross section in collisions between fullerenes requires an extended analysis of the collision trajectories $\mathbf{R}(t)$. Contrary to ion-atom collisions, where the straight-line trajectory approximation provides an excellent description of the majority of experiments, the trajectories of nanoparticles may be strongly influenced by the excitation of the nanoparticles' internal structures and by the formation of long-lived intermediate complexes. This change in trajectory becomes especially important for explaining the large scattering angle contribution to the total charge-transfer cross section.

Modeling average trajectory. The collision dynamics depend on the impact parameter and collision energy. Within the interval of experimental velocities reported in Glotov and Campbell [16], the fullerene collisions exhibit small scattering angles if the impact parameters are larger than the C_{60} diameter $d = 13.33$ bohr radii a_0 [27]. This implies a relatively small value of the exchange phase $\Phi(v, b) < 1$ and so a small probability $P(v, b)$, similar to what is usually observed in ion-atom collisions. If the impact parameter is less than the diameter d, the average probability of charge transfer $\langle P(v, b)\rangle \simeq 1/2$, due to the large value of the exchange interaction and exchange phase $\Phi(v, b)$. This reflects the overlap of the internal structures of the colliding particles. The contribution to the charge-transfer cross section for $b < d$ is therefore estimated as $\sigma_c \simeq 0.5\pi d^2$. Finally, when $b \sim d$ we expect the formation of temporary chemical bonds, or "bridges," between fullerenes. These bridges, and the transfer of the collision energy into the fullerenes' internal degrees of freedom, extend the time of interaction between the fullerenes at low collision velocities. Colliding fullerenes can form a long-lived dumbbell-shaped $(C_{60} - C_{60})^+$ quasimolecule. The lifetime of this state and the structure of this state depends on the collision velocity, which affects the probability of charge transfer between the fullerenes.

To visualize the mechanism for the formation of temporary chemical bonds, we performed QMD simulations of $C_{60} + C_{60}{}^+$ collisions at different velocities and impact parameters. Our simulations were performed using the atom-centered density-matrix propagation (ADMP) method [28] as implemented in the GAUSSIAN 16 electronic structure programs [29]. The electronic energy and its gradient are computed using the PM3 semiempirical method [30,31].

The translational energy loss and collision time delay have been investigated at different impact parameters and at collision energies in the range from around 1 eV up to several hundred eV. In Fig. 2 the kinetic energy of all 120 carbon atoms is shown as a function of time from one of our simulations. This simulation is at a collision energy of 409 eV and an impact parameter of $b = 14.17a_0$, which is slightly larger than the C_{60} diameter d. In this relatively fast collision, the overlap of electronic states of different fullerenes is not enough to establish long-lived bonds between the fullerenes and so only 3% of the translational kinetic energy is lost to the internal energies of the C_{60} molecules. We found that the relative loss of translational energy is only significant for impact parameters below the diameter of C_{60} and has only a slight dependence on collision velocities at higher collision energies. For collisions with an energy on the order of 1 eV, the interaction time between fullerenes is sufficiently long enough to establish "bridges" and the loss of the translational energy increases. The formation of bridges and the formation of long-lived quasimolecules has been observed at these lower collision velocities. The effective number of bridges and the time delay associated with the formation of intermediate $(C_{60} - C_{60})^+$ states decrease with an increase of collision velocities and have been hardly seen at velocities above 2×10^4 m/s.

Based on our QMD simulations and the results of other simulations [20–22], the chemical bonds of C_{60} molecules do not stretch significantly during collisions at the considered velocities. The molecules mostly experience temporary compression and temporary deformation during their close encounter. In order to include the compression of the molecules in our model, while we calculate the splitting between the gerade and ungerade states as a function of the intermolecular distance R, we forced the atoms to never be closer than 1 Å.

Key to our model is the prediction that temporary bonds between fullerenes significantly increase the probability of charge transfer. The time $\tau(v, b)$ of the interaction between two colliding C_{60} fullerenes, also known as the collision time delay, is a function of both the velocity v and impact parameter b, and it can be determined as

$$\tau(E, b) = 2\frac{d\eta_r(E, b)}{dE} + 2\frac{d\eta_c(E, b)}{dE}, \tag{6}$$

where $\eta_r(E, b)$ and $\eta_c(E, b)$ are the Breit-Wigner resonance and background scattering phases, respectively [32], and E is the collision energy. During collisions involving fullerenes, the formation of dumbbell quasimolecules occur in various excited states with different configurations. Therefore, we expect several Breit-Wigner resonances arising at different resonance velocities v_i. The following simplified empirical formula can be used for the evaluation of the collision time delay and thus the lifetime of the temporary chemical bonds,

$$\tau(v, b) = \sum_i a_i(b)\frac{\gamma_{i_c}}{\left(v^2 - v_i^2\right)^2 + \gamma_i^2} + \tau_c(v, b), \tag{7}$$

where the first term is the sum of the Breit-Wigner resonances describing the formation of various long-lived states of the quasimolecule $(\mathrm{C}_{60} - \mathrm{C}_{60})^+$ with a total resonance width $\gamma_i(b)$. In multichannel scattering, the partial width $\gamma_{i_c}(b)$ corresponds to the resonant charge-transfer channel and the factor $a_i(b)$ takes into account the dependence of the relative strength of resonances on the impact parameter b. In the vicinity of resonance, the dependence of the background scattering time delay $\tau_c(v, b)$ on the velocity and impact parameter can be neglected.

For the considered collision velocities, the trajectories of the particles are straight lines, $R(t) = \sqrt{b^2 + v^2t^2}$, for most of the collision. Accurate trajectories need to take into account the time delay $\tau(v, b)$ due to the temporary formation of quasimolecules. The exponential decay of the quasimolecules with the characteristic time $\tau(v, b)$, corresponds to the Breit-Wigner resonance formula. The average rate of change $v(t)$ of the interparticle distance can be represented as $v(t) = v(1 - e^{-|t|/\tau(v,b)})$, where v is the collision velocity. Since the absolute value of time is used, this equation assumes that the same time is required for the formation of and for the spontaneous decay of the quasimolecule state. Therefore, the trajectories of $R(t)$ can be approximated by the following equation:

$$R(t) = \sqrt{b^2 + v^2t^2(1 - e^{-|t|/\tau(v,b)})^2}. \tag{8}$$

This function approaches v as t approaches either negative infinity or positive infinity, meaning that at large distances R the trajectory returns to the original straight-line trajectory.

Results. The experimental data of the charge-transfer cross sections [16] were measured for the interval of collision velocities $v > v_i$ where the time delay is not expected to be very large, and τ may be approximated using only a single resonance v_i with no background time delay τ_c. This single resonant velocity was fit to the data and found to be 9×10^3 m/s. The width of the resonance γ_i was also fit to the data and found to be 5×10^2 m^2/s^2. The factor $a_i(b)$ was taken to be $1/b^2$. γ_{i_c} was fit as well and was $\gamma_{i_c} = 300a_0^2$ m^4/s^3. The effective size of the zero-range potentials in our model was set to $\kappa = 0.85$ hartree$^{1/2}$. For collisions with $b < d$ we estimated the charge-transfer cross section as $\sigma_c \simeq 0.5\pi d^2$. This core cross section should not be sensitive to the collision velocity. It corresponds to trajectories with large scattering angles and large recoil energy losses observed in the measurement of fast neutral products [16]. The solid curves in Fig. 3 show the results of our model, which does account for the formation of quasimolecules, for both the small scattering angle cross section (lower curve) and total charge-transfer cross section (upper curve). Figure 3 also shows the experimental data for both the small scattering angle charge transfer cross section [15] and the total charge transfer cross section [16]. The lower dashed curve is the small scattering angle cross section computed using the electron wave function from the jellium model of C_{60} and the Holstein-Herring method [19]. By assuming the probability of charge transfer is $1/2$ for all impact parameters below the diameter of C_{60}, d, this cross section was shifted up, shown as the upper dashed curve. This simplified model, which does not extend the interaction time in order to account for the formation of quasimolecules, does not fit well to the data at lower collision velocities. Results of our ZRP model calculations (the solid curves) are in very good agreement with the experimental data.

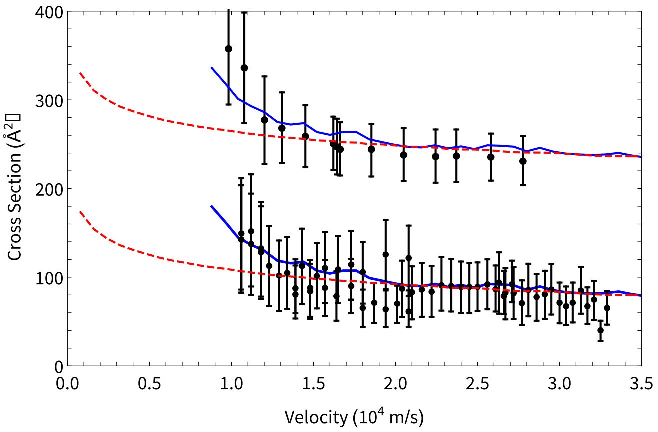

FIG. 3. Data from Glotov and Campbell [16] (shown as black dots) alongside our models. The upper part of the graph represents the total cross section and the lower part represents the small scattering angle cross section. The two solid curves are our model accounting for the extended interaction time due to a temporary "bridge" formation. The two dashed curves represent our model without accounting for the bridge formation.

The available experimental data [16] can illustrate only a marginal increase of the cross sections due to the formation of long-lived compound quasimolecules in collisions of two fullerenes. We predict that the Breit-Wigner resonances at low collision velocities support long-lived bridges between fullerenes and this leads to a significant increase in the charge-transfer cross sections. Direct experimental measurements of $\mathrm{C}_{60} + \mathrm{C}_{60}{}^+$ charge transfer and scattering cross sections at energies of several eV would be an important test of the bridge model and for the formation of the intermediate compound states in collisions of slow fullerenes.

Conclusion. An efficient computational model has been developed to explain experimental data on the cross section of $\mathrm{C}_{60} + \mathrm{C}_{60}{}^+$ resonant charge-transfer collisions. In this model, the electronic state of the C_{60} active electron is described by an electron bound by 60 identical zero-range potentials evenly distributed across the C_{60} molecule. The Hamiltonian of the colliding fullerenes is reduced to the corresponding 120×120 matrix that describes the electronic state of the quasimolecule formed in the $C_{60} + C_{60}{}^{+}$ collision. The electronic states of the quasimolecule are computed for different time-dependent distances between colliding particles. The proposed model of the charge-transfer process accounts for the formation of temporary chemical bonds between colliding fullerenes. These bonds significantly extend the interparticle exchange interaction. We predict that at lower collision energies the charge exchange between fullerenes is controlled by the Breit-Wigner resonances arising due to a temporary creation of a dumbbell-shaped quasimolecule $(C_{60} - C_{60})^{*+}$. The formation of long-lived quasimolecules have been also observed in our QMD simulations. Results of the calculated resonant charge-transfer cross section in $C_{60} + C_{60}{}^{+}$ collisions are in good agreement with the experimental data.

Acknowledgments. R.C. was supported by the National Science Foundation (NSF) Grant No. PHY-2034284. V.K. acknowledges support from the NSF through a grant for ITAMP at Center for Astrophysics | Harvard & Smithsonian.

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