

Subfemtosecond charge dynamics in vertically stacked bilayer silicene

Junais Habeeb Mokkath 

Quantum Nanophotonics Simulations Lab,
Department of Physics, Kuwait College of
Science and Technology, Doha, Kuwait

Correspondence

Junais Habeeb Mokkath, Quantum
Nanophotonics Simulations Lab, Department
of Physics, Kuwait College of Science and
Technology, Doha Area, 7th Ring Road,
P.O. Box 27235, Doha, Kuwait.
Email: j.mokkath@kcst.edu.kw

Funding information

Kuwait College of Science and Technology
(KCST)

Abstract

Ultrafast charge dynamics in two-dimensional materials have attracted great interest from both fundamental and applied perspectives due to its significance in the next-generation battery and solar cells. In this work, using the realistic quantum mechanical real-time propagation time-dependent density functional theory (*rt*-TDDFT) simulations, we disclose the ultrafast charge dynamics in vertically stacked bilayer silicene subjected to an external bias. Among other insights, our study indicates that even modest changes in interlayer distance produce significant modulations in the ultrafast charge dynamics at the subfemtosecond time scale. The findings in this work may open new pathways for the use of bilayer silicene in novel optoelectronic and photovoltaic devices.

KEYWORDS

bilayer silicene, *rt*-TDDFT, ultrafast charge dynamics

1 | INTRODUCTION

More recently, there has been an increasing research effort to find two-dimensional (2D) materials and the possibility to combine them in vertical stacks.^[1-8] While the structure of traditional 2D materials is limited by the strict requirement of lattice matching between constituent materials (in order to preclude defect formation and large strain at the interface), such problems are substantially reduced in the van der Waals structures consisting of 2D materials. In this context, graphene (an atomically thin layer of honeycomb C atoms) has inspired much interest due to its astonishing electronic, optical, and mechanical properties.^[9-18] Inspired by the findings based on graphene, recently, much interest has been paid to silicene (Si atoms packed in a honeycomb lattice).^[19-31] Silicene can exist with a mixed sp^2/sp^3 ratio and with a variety of lattice constants. This structural flexibility in silicene created significant opportunities for exploring novel physics and ground-breaking applications. From a technological point of view, the compatibility of silicene with the silicon-based nanotechnology industry makes it particularly interesting for device applications.

In a related context, a fundamental understanding of the ultrafast charge dynamics in 2D materials at the subfemtosecond time scale offers unprecedented opportunities in nanoscale charge transport and helps the rational design of high-performance optoelectronic and photocatalytic devices.^[32-42] First-principles calculations have long been used successfully to obtain comprehensive insight and detailed knowledge of the charge dynamics at the atomic scale. One such routinely exploited technique is a hybrid methodology, which combines the density functional theory (DFT) and nonequilibrium Green's functions (NEGF).^[43-49] However, despite the widespread use of "DFT + NEGF" formalism to characterize the charge dynamics at the atomic scale, it is static, with dynamic response incorporated through complicated extensions. Nevertheless, rapid advancements in ultrafast techniques have enabled a large number of excited-state phenomena to be observed in real time and demand the use of a dynamic (time-dependent) technique, such as the real-time propagation time-dependent density functional theory (*rt*-TDDFT).^[50-59] It is based on time evolution of the occupied Kohn-Sham orbitals under an intense electromagnetic pulse. This is a powerful technique capable of providing an excellent ratio of accuracy over computational cost and is highly successful in dealing with large systems composed of thousands of electrons or hundreds of atoms.^[55-61] The possibility of obtaining the response of the system with femtosecond resolution, as well as the flexibility to decouple the effects of electronic and nuclear response, makes the *rt*-TDDFT simulations complementary to laboratory observations.

The purpose of the present paper is to theoretically demonstrate the modulations in the ultrafast charge dynamics in vertically stacked bilayer silicene^[62-70] as a function of the interlayer distance. We report novel results that have not been seen before in bilayer silicene, particularly dramatic modulation in subfemtosecond charge dynamics. The paper is organized as follows. In the section that follows, we outline the computational system and computational techniques employed. We show our results and discuss them in the next section, specifically addressing the modulations in the unbiased charge density, biased charge density, and current in the middle, between layers. The conclusions and outlook section closes the paper.

2 | COMPUTATIONAL ASPECTS

All calculations in this work were performed using the *rt*-TDDFT code implemented in the open-source Quantum Espresso software package.^[71] We note that the *rt*-TDDFT method is rapidly gaining prominence as it is one of the few computationally affordable ways to model ultrafast charge dynamics in periodic materials.^[51,72,73] An important advantage of using *rt*-TDDFT is its capability to render the full-frequency dependence of properties of interest via a Fourier transform from the time domain to the frequency domain. Furthermore, with many k-points sampling the reciprocal space, a relatively small computational cell is needed to simulate quantum phenomena for a long time and renders essential information

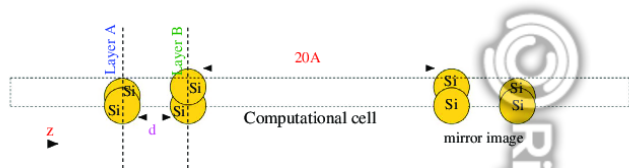


FIGURE 1 Schematic representation of the computational supercells used for DFT and *rt*-TDDFT calculations

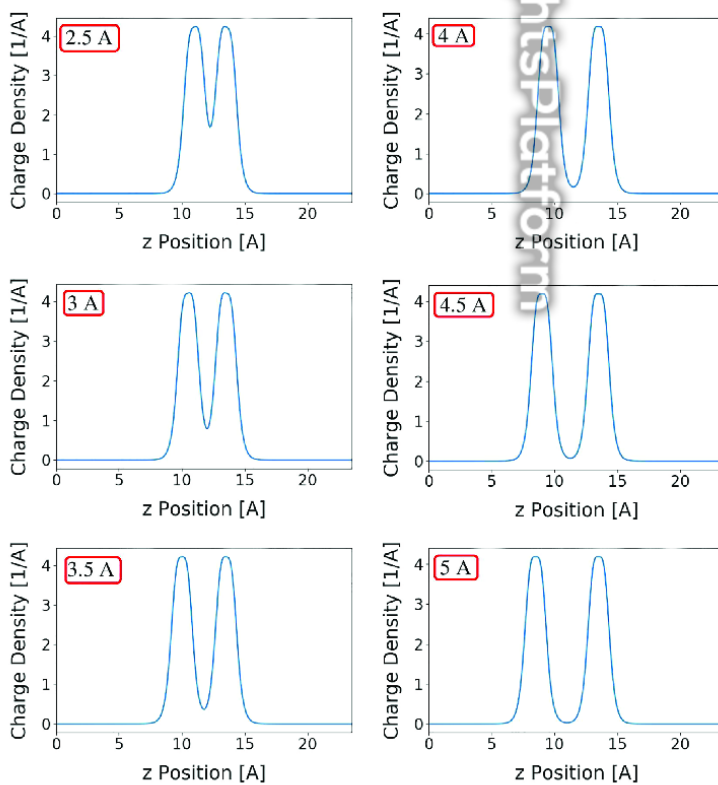


FIGURE 2 Ground-state charge density of a vertically stacked bilayer silicene along the *z* direction as a function of the interlayer distance (*d*) in the range of 2.5 to 5 Å

concerning the real-time evolution of electron density fluctuations. Regarding the DFT and *rt*-TDDFT simulations, we adopted the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation^[74] to describe the exchange-correlation energy. The wave functions are expanded in a plane wave basis set with an energy cutoff of 400 eV. The Brillouin zone of the bilayer silicene was sampled with a Γ -centered grid, with a *k*-point density corresponding to $17 \times 17 \times 1$ *k*-points in the primitive cell. The self-consistency tolerance of the total energy is fixed to 10^{-7} eV/atom. Our computational cell (see Figure 1) comprises a vertically stacked bilayer silicene, with the interlayer distance *d* varying in the range of 2.5 to 5 Å in small increments of 0.5 Å. We note that the ultrafast charge transfer is sensitive to the interlayer electronic coupling, and naively, one would expect that the shorter the interlayer distance is, the faster the interlayer charge transfer will be. Each of the layers (layer A and layer B) consists of two Si atoms. The fictitious dipole moment is counteracted with a mirror image (located at a distance of 20 Å from layer B, see Figure 1). We did not optimize the structures as a whole during the *rt*-TDDFT simulations as we wanted to elucidate the modulations in the ultrafast charge transfer as a function of the interlayer distance while keeping all other geometrical parameters unchanged. During the *rt*-TDDFT simulations, the excited wave function was propagated for 1000 steps via the Crank-Nicholson propagator^[75] with strict conservation of the total charge. We propagate the system for the total propagation time of 1 femtosecond and a time step of 1 attosecond. Finally, the quantities of interest, such as the current and voltage decay, were calculated.

3 | RESULTS AND DISCUSSION

We start the discussion by analyzing the modulations in the (unbiased) ground-state charge density for a vertically stacked bilayer silicene along the *z* direction as a function of the interlayer distance (*d*) in the range of 2.5 to 5 Å (see Figure 2). One finds a systematic modulation in the ground-state charge density with the increasing value of the interlayer distance (*d*). Note that, in the case of *d* = 4.5 and 5 Å, layer A and layer B are sufficiently apart from each other, and the resulting overlap of the individual charge densities is negligible. Now, let us analyze the modulations in the charge density profiles, starting from *d* = 2.5 Å. Figure 2 shows that, for *d* = 2.5 Å, layer A is located at *z* = 11 Å, and layer B is located at

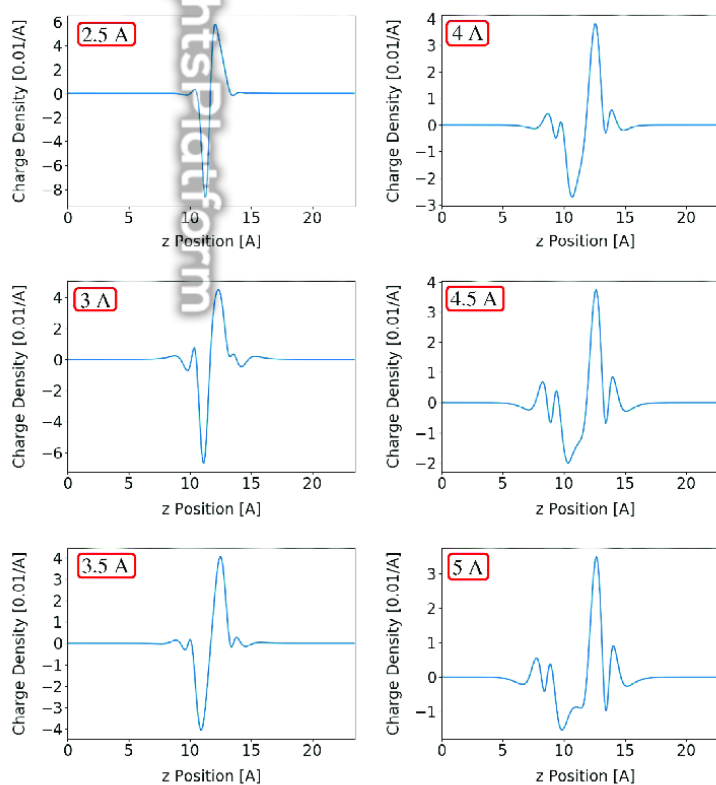


FIGURE 3 Biased ground-state charge density of a vertically stacked bilayer silicene along the *z* direction as a function of the interlayer distance (*d*) in the range of 2.5 to 5 Å. We note that -0.5 V is applied to layer A, and 0.5 V is applied to layer B. The plots illustrate how electrons are dragged from layer A to layer B by the bias voltage

$z = 13.5 \text{ \AA}$. As expected, there is a significant overlap of the charge densities in the middle of the junction. In the case of $d = 3 \text{ \AA}$, layer A is located at $z = 10.5 \text{ \AA}$, and layer B is located at $z = 13.5 \text{ \AA}$. Apparently, the overlap between the charge densities is now somewhat reduced (in comparison to $d = 2.5 \text{ \AA}$), and the sharp dip in the charge density profile in the middle of the junction is more significant. Furthermore, it is worth noting that the dip in the charge density profile is further shifted down in the case of $d = 4 \text{ \AA}$, suggesting that the charge density overlap between layers A and B is further reduced. This scenario is substantially changed starting from $d = 4.5 \text{ \AA}$, where layer A is located at $z = 9 \text{ \AA}$, and layer B is located at $z = 13.5 \text{ \AA}$; see Figure 2. Interestingly, one finds that the individual charge densities are now clearly separated to the left and right, and there is no overlap in the middle of the junction. A similar observation is valid in the case of $d = 5 \text{ \AA}$ as well.

Having discussed/analyzed how the (unbiased) ground-state charge density of a vertically stacked bilayer silicene along the z direction changes as a function of the interlayer distance (d) in the range of 2.5 to 5 \AA , we now turn our attention to a similar analysis but with -0.5 V applied to layer A and 0.5 V applied to layer B; see Figure 3. Simply put, these plots demonstrate how electrons are dragged from layer A to layer B by the applied bias voltage. Figure 3 shows that there is a systematic reduction in the number of transferred electrons from layer A to layer B, with the increase in the d value in the range of 2.5 to 5 \AA . In addition, there is a dramatic modulation in the charge density profiles with respect to the d variations. For d in the range of 2.5 to 4 \AA , the biased charge densities of layer A and layer B are almost symmetrically distributed; see Figure 3. Remarkably, the situation quickly changes in the case of $d = 4.5$ and 5 \AA . Note that their biased charge densities are more unsymmetrical. This is because the transferred electrons from layer A do not reach (fully) layer B.

After understanding both unbiased and biased ground-state charge densities of a vertically stacked bilayer silicene along the z direction as a function of d , we further explore the decay of the bias voltage and the resulting current in the middle of the junction between layer A and layer B; see Figure 4. Our preliminary analysis reveals some impressive results; in particular, Figure 4 illustrates a discharging mechanism analogous to a parallel plate capacitor. On the other hand, Figure 4 shows that the maximum value of the current (I_{max}) appears at 400 attoseconds (0.4 femtosecond) for all d values, except for $d = 2.5 \text{ \AA}$ where the I_{max} appears at 60 attoseconds (0.06 femtosecond). This significant reduction in the I_{max} value for $d = 2.5 \text{ \AA}$ is likely due to the strong charge density overlap. Overall, we note that the decay of the current displays systematic trends as a

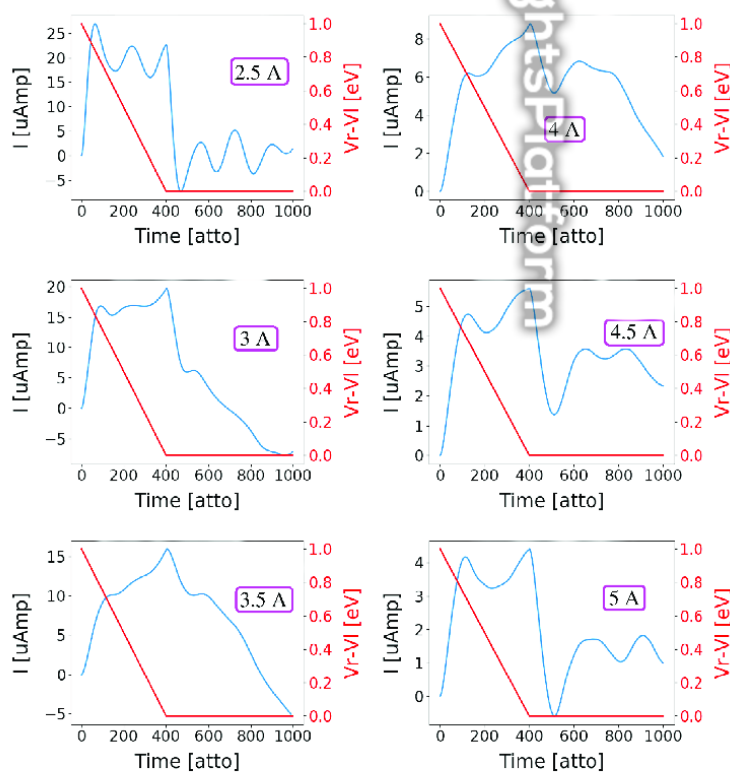


FIGURE 4 The decay of the external bias voltage and the resulting current at the middle between layer A and layer B. Note that -0.5 V is applied to layer A, and 0.5 V is applied to layer B

function of the increasing d values. Now, let us analyze the outcomes in detail. For $d = 3 \text{ \AA}$, there is a dramatic modulation in the current values. In particular, I_{max} appears at 400 attoseconds, and the current becomes 0 \mu A at 650 attoseconds. In the case of $d = 3.5 \text{ \AA}$, I_{max} again appears at 400 attoseconds; however, the current becomes 0 \mu A at 850 attoseconds. In the case of $d = 4$ and 4.5 \AA , the current value never becomes 0. Finally, in the case of $d = 5 \text{ \AA}$, the current value becomes 0 \mu A at 480 attoseconds. Remarkably, the results shown in Figure 4 indicate that vertically stacked bilayer silicene can be considered atomically thin nanocapacitors with significantly distinct discharging features simply by tuning the thickness of the junction region. The variations in the discharging features can be attributed to the many quantum features, including the kinetic energy of the electrons, exchange energy, and correlation energy.^[76]

In what follows, we focus on the subfemtosecond discharging process in the middle between layer A and layer B via heatmaps; see Figure 5. We note that the heatmaps can explain the subfemtosecond discharging process in more detail through an easy and fast two-dimensional visualization. In the case of $d = 2.5 \text{ \AA}$, the current predominantly flows from layer A to layer B for up to 400 attoseconds. After this, the current follows an oscillatory behavior, suggesting that the current flows in both directions. Similar conclusions can also be drawn in the case of $d = 3 \text{ \AA}$. Nevertheless, a different scenario emerges for $d = 3.5 \text{ \AA}$. In particular, the discharging time is now slightly increased. A more dramatic situation occurs in the case of $d = 4$ and 4.5 \AA . We observe that the current is now able to be sustained for longer, up to 1000 attoseconds (one femtosecond). Finally, in the case of $d = 5 \text{ \AA}$, current flows from layer A to layer B for up to 400 attoseconds (0.4 femtosecond). These results capture well the data shown in Figure 4. Finally, it is worth mentioning that doubling the number of atoms in layer A and layer B produced more or less similar results in comparison to the system where layer A and layer B consist of two atoms each; see Figure 6. Overall, based on the findings in this paper, one can favorably manipulate the ultrafast charge dynamics in vertically stacked bilayer silicene. The present results could open new avenues to design future applications of bilayer silicene in novel optoelectronic and light-harvesting devices.

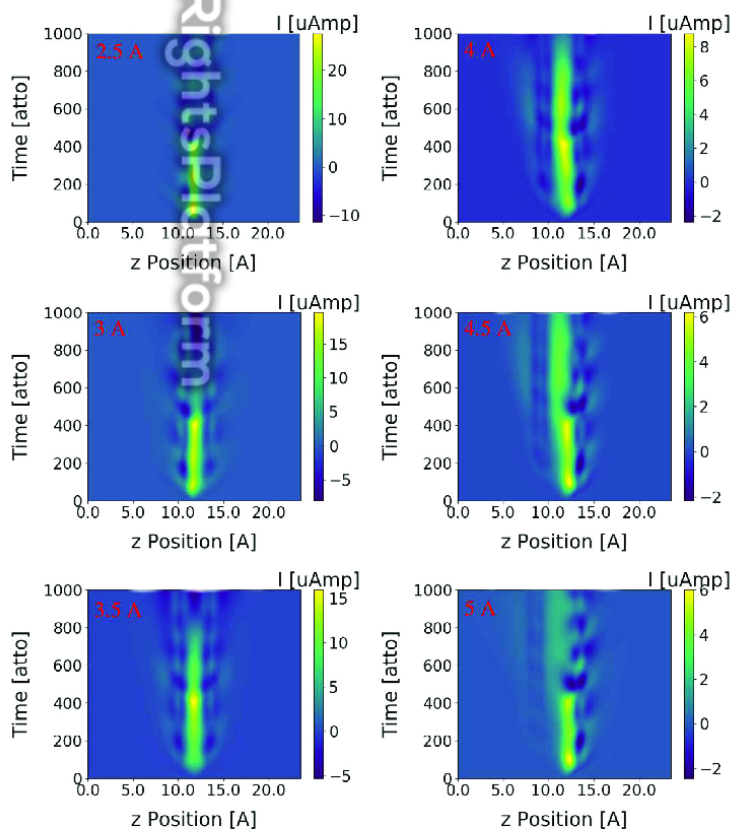


FIGURE 5 Heatmaps demonstrating the discharging current in the middle between layer A and layer B for d in the range of 2.5 to 5 \AA . At time = 0 attosecond, an equilibrium ground state is achieved, with layer A gated at -0.5 V and layer B gated at 0.5 V . After unsetting this bias voltage, a discharging current flows back to layer B

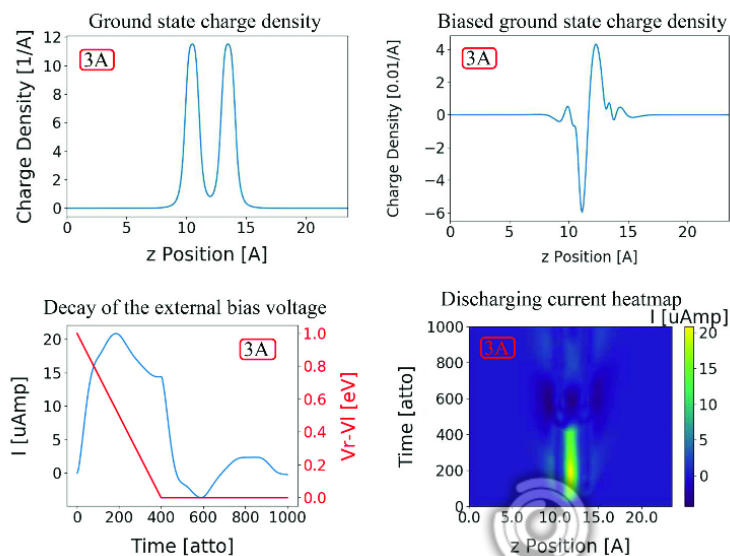


FIGURE 6 Ground-state charge density, biased ground-state charge density, decay of the external bias voltage, and discharging current heatmap of a vertically stacked bilayer silicene (with layer A and layer B, consisting of four atoms each) for $d = 3 \text{ \AA}$

4 | CONCLUSIONS AND OUTLOOK

Understanding ultrafast charge dynamics in 2D materials helps the design of high-performance optoelectronic devices. Here, we thoroughly investigated the ultrafast charge dynamics of a vertically stacked bilayer silicene as a function of the interlayer distances at proximity using the realistic quantum mechanical *rt*-TDDFT calculations. We found a strong interlayer distance dependence of ultrafast charge dynamics at the sub-femtosecond time scale. We hope that the findings in this theoretical study provide the opportunity for further investigations on ultrafast charge dynamics in vertically stacked bilayer silicene.

ACKNOWLEDGEMENTS

The research reported in this publication was supported by funding from Kuwait College of Science and Technology (KCST).

AUTHOR CONTRIBUTIONS

Junais Habeeb Mokkath: Conceptualization; data curation; formal analysis; funding acquisition; investigation; methodology; project administration; resources; software; supervision; validation; visualization; writing-original draft; writing-review and editing.

ORCID

Junais Habeeb Mokkath  <https://orcid.org/0000-0001-8889-5889>

REFERENCES

- [1] A. K. Geim, I. V. Grigorieva, *Nature* **2013**, *499*, 419.
- [2] A. J. Frenzel, C. H. Lui, Y. C. Shin, J. Kong, N. Gedik, *Phys. Rev. Lett.* **2014**, *113*, 056602.
- [3] H. Wang, C. Zhang, F. Rana, *Nano Lett.* **2015**, *15*, 339.
- [4] K. F. Mak, C. Lee, J. Hone, J. Shan, T. F. Heinz, *Phys. Rev. Lett.* **2010**, *105*, 136805.
- [5] A. Splendiani, L. Sun, Y. Zhang, T. Li, J. Kim, C.-Y. Chim, G. Galli, F. Wang *Nano Lett.* **2010**, *10*, 1271.
- [6] A. F. Rigosi, H. M. Hill, Y. Li, A. Chernikov, T. F. Heinz, *Nano Lett.* **2015**, *15*, 5033.
- [7] L. Zhang, A. Zunger, *Nano Lett.* **2015**, *15*, 949.
- [8] S. W. Han, H. Kwon, S. K. Kim, S. Ryu, W. S. Yun, D. H. Kim, J. H. Hwang, J.-S. Kang, J. Baik, H. J. Shin, S. C. Hong, *Phys. Rev. B* **2011**, *84*, 045409.
- [9] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, *Science* **2004**, *306*, 666.
- [10] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, A. A. Firsov, *Nature* **2005**, *438*, 197.
- [11] A. K. Geim, K. S. Novoselov, *Nat. Mater.* **2007**, *6*, 183.
- [12] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, A. K. Geim, *Rev. Mod. Phys.* **2009**, *81*, 109.
- [13] Y. Zhang, Y.-W. Tan, H. L. Stormer, P. Kim, *Nature* **2005**, *438*, 201.

- [14] C. Berger, Z. Song, X. Li, X. Wu, N. Brown, C. Naud, D. Mayou, T. Li, J. Hass, A. N. Marchenkov, E. H. Conrad, P. N. First, W. A. de Heer, *Science* **2006**, *312*, 1191.
- [15] W. Choi, I. Lahiri, R. Seelaboyina, Y. S. Kang, *Crit. Rev. Solid State Mater. Sci.* **2010**, *35*, 52.
- [16] B. Hunt, J. D. Sanchez-Yamagishi, A. F. Young, M. Yankowitz, B. J. LeRoy, K. Watanabe, T. Taniguchi, P. Moon, M. Koshino, P. Jarillo-Herrero, R. C. Ashoori, *Science* **2013**, *340*, 1427.
- [17] M. Zhu, D. Ghazaryan, S.-K. Son, C. R. Woods, A. Misra, L. He, T. Taniguchi, K. Watanabe, K. S. Novoselov, Y. Cao, A. Mishchenko, *2D Mater.* **2016**, *4*, 011013.
- [18] S. J. Ahn, P. Moon, T.-H. Kim, H.-W. Kim, H.-C. Shin, E. H. Kim, H. W. Cha, S.-J. Kahng, P. Kim, M. Koshino, Y.-W. Son, C.-W. Yang, J. R. Ahn, *Science* **2018**, *361*, 782.
- [19] L. Chen, C.-C. Liu, B. Feng, X. He, P. Cheng, Z. Ding, S. Meng, Y. Yao, K. Wu, *Phys. Rev. Lett.* **2012**, *109*, 056804.
- [20] M. Houssa, G. Pourtois, V. V. Afanas'ev, A. Stesmans, *Appl. Phys. Lett.* **2010**, *97*, 112106.
- [21] H. Jamgotchian, Y. Colignon, N. Hamzaoui, B. Ealet, J. Y. Hoarau, B. Aufray, J. P. Bibérian, *J. Phys.: Condens. Matter* **2012**, *24*, 172001.
- [22] B. Feng, Z. Ding, S. Meng, Y. Yao, X. He, P. Cheng, L. Chen, K. Wu, *Nano Lett.* **2012**, *12*, 3507.
- [23] R. Arafune, C.-L. Lin, K. Kawahara, N. Tsukahara, E. Minamitani, Y. Kim, N. Takagi, M. Kawai, *Surf. Sci.* **2013**, *608*, 297.
- [24] M. Houssa, A. Dimoulas, A. Molle, *J. Phys.: Condens. Matter* **2015**, *27*, 253002.
- [25] J. Zhuang, X. Xu, H. Feng, Z. Li, X. Wang, Y. Du, *Sci. Bull.* **2015**, *60*, 1551.
- [26] S. Cahangirov, H. Sahin, G. Le Lay, A. Rubio, *Lecture Notes in Physics*, Springer, Berlin **2017**.
- [27] A. Molle, C. Grazianetti, L. Tao, D. Taneja, M. H. Alam, D. Akinwande, *Chem. Soc. Rev.* **2018**, *47*, 6370.
- [28] J. H. Makkath, U. Schwingenschlöggl, *J. Mater. Chem. C* **2016**, *4*, 7387.
- [29] H. Şahin, S. Cahangirov, M. Topsakal, E. Bekaroglu, E. Akturk, R. T. Senger, S. Ciraci, *Phys. Rev. B* **2009**, *80*, 155453.
- [30] Z. Ni, Q. Liu, K. Tang, J. Zheng, J. Zhou, R. Qin, Z. Gao, D. Yu, J. Lu, *Nano Lett.* **2012**, *12*, 113.
- [31] P. De Padova, O. Kubo, B. Olivieri, C. Quaresima, T. Nakayama, M. Aono, G. Le Lay *Nano Lett.* **2012**, *12*, 5500.
- [32] J. Zhang, H. Hong, C. Lian, W. Ma, X. Xu, X. Zhou, H. Fu, K. Liu, S. Meng, *Adv. Sci.* **2017**, *4*, 1700086.
- [33] S. M. Falke, C. A. Rozzi, D. Brida, M. Maiuri, M. Amato, E. Sommer, A. De Slo, A. Rubio, G. Cerullo, E. Molinari, C. Lienau, *Science* **2014**, *344*, 1001.
- [34] C. Andrea Rozzi, S. Maria Falke, N. Spallanzani, A. Rubio, E. Molinari, D. Brida, M. Maiuri, G. Cerullo, H. Schramm, J. Christoffers, C. Lienau, *Nat. Commun.* **2013**, *4*, 1602.
- [35] X. Hong, J. Kim, S.-F. Shi, Y. Zhang, C. Jin, Y. Sun, S. Tongay, J. Wu, Y. Zhang, F. Wang, *Nat. Nanotechnol.* **2014**, *9*, 682.
- [36] R. Long, O. V. Prezhdo, *Nano Lett.* **2016**, *16*, 1996 26882202.
- [37] Y. Shi, O. V. Prezhdo, J. Zhao, W. A. Saidi, *ACS Energy Lett.* **2020**, *5*, 1346.
- [38] Q. Zheng, Y. Xie, Z. Lan, O. V. Prezhdo, W. A. Saidi, J. Zhao, *Phys. Rev. B* **2018**, *97*, 205417.
- [39] C. Jin, E. Y. Ma, O. Karni, E. C. Regan, F. Wang, T. F. Heinz, *Nat. Nanotechnol.* **2018**, *13*, 994.
- [40] Y. Garcia-Basabe, A. R. Rocha, F. C. Vicentin, C. E. P. Villegas, R. Nascimento, E. C. Romani, E. C. de Oliveira, G. J. M. Fecine, S. Li, G. Eda, D. G. Larrude, *Phys. Chem. Chem. Phys.* **2017**, *19*, 29954.
- [41] A. Boulesbaa, K. Wang, M. Mahjouri-Samani, M. Tian, A. A. Puzos, I. Ivanov, C. M. Rouleau, K. Xiao, B. G. Sumpter, D. B. Geohegan *J. Am. Chem. Soc.* **2016**, *138*, 14713.
- [42] T. Suzuki, T. Iimori, S. J. Ahn, Y. Zhao, M. Watanabe, J. Xu, M. Fujisawa, T. Kanai, N. Ishii, J. Itatani, K. Suwa, H. Fukidome, S. Tanaka, J. R. Ahn, K. Okazaki, S. Shin, F. Komori, I. Matsuda, *ACS Nano* **2019**, *13*, 11981.
- [43] J. J. Palacios, A. J. Pérez-Jiménez, E. Louis, E. SanFabian, J. A. Vergés, *Phys. Rev. B* **2002**, *66*, 035322.
- [44] J. Taylor, H. Guo, J. Wang, *Phys. Rev. B* **2001**, *63*, 245407.
- [45] S.-H. Ke, H. U. Baranger, W. Yang, *Phys. Rev. B* **2004**, *70*, 85410.
- [46] D. A. Areshkin, B. K. Nikolić, *Phys. Rev. B* **2010**, *81*, 155450.
- [47] X. Hu, H. Qu, L. Xu, W. Liu, T. Guo, B. Cai, X. Yu, J. Zhu, S. Zhang, *Nanoscale* **2020**, *12*, 9958.
- [48] Y. Xue, S. Datta, M. A. Ratner, *Chem. Phys.* **2002**, *281*, 151.
- [49] M. Brandbyge, J.-L. Mozos, P. Ordejón, J. Taylor, K. Stokbro, *Phys. Rev. B* **2002**, *65*, 165401.
- [50] K. Yabana, G. F. Bertsch, *Phys. Rev. B* **1996**, *54*, 4484.
- [51] K. Yabana, T. Nakatsukasa, J.-I. Iwata, G. F. Bertsch, *Phys. Status Solidi* **2006**, *243*, 1121.
- [52] T. Sander, G. Kresse, *J. Chem. Phys.* **2017**, *146*, 064110.
- [53] J. Jorner-Somoza, J. Alberdi-Rodríguez, B. F. Milne, X. Andrade, M. A. L. Marques, F. Nogueira, M. J. T. Oliveira, J. J. P. Stewart, A. Rubio, *Phys. Chem. Chem. Phys.* **2015**, *17*, 26599.
- [54] J. H. Makkath, U. Schwingenschlöggl, *J. Phys. Chem. C* **2013**, *117*, 23938.
- [55] J. Theilhaber, *Phys. Rev. B* **1992**, *46*, 12990.
- [56] Y. Takimoto, F. D. Vila, J. J. Rehr, *J. Chem. Phys.* **2007**, *127*, 154114.
- [57] C. M. Isborn, X. Li, *J. Chem. Theory Comput.* **2009**, *5*, 2415.
- [58] F. Ding, B. E. Van Kuiken, B. E. Eichinger, X. Li, *J. Chem. Phys.* **2013**, *138*, 064104.
- [59] B. Peng, D. B. Lingerfelt, F. Ding, C. M. Aikens, X. Li, *J. Phys. Chem. C* **2015**, *119*, 6421.
- [60] S. Tussupbayev, N. Govind, K. Lopata, C. J. Cramer, *J. Chem. Theory Comput.* **2015**, *11*, 1102.
- [61] V. Alejandro, G.-G. Pablo, F. Johannes, F. J. Garcia-Videl, R. Angel, *Nanophotonics* **2016**, *5*, 3.
- [62] M. Ezawa, *J. Phys. Soc. Jpn.* **2012**, *81*, 104713.
- [63] C. Lian, J. Ni, *AIP Adv.* **2013**, *3*, 052102.
- [64] B. Huang, H.-X. Deng, H. Lee, M. Yoon, B. G. Sumpter, F. Liu, S. C. Smith, S.-H. Wei, *Phys. Rev. X* **2014**, *4*, 021029.
- [65] F. Liu, C.-C. Liu, K. Wu, F. Yang, Y. Yao, *Phys. Rev. Lett.* **2013**, *111*, 066804.
- [66] J. E. Padilha, R. B. Pontes, *J. Phys. Chem. C* **2015**, *119*, 3818.
- [67] P. De Padova, P. Vogt, A. Resta, J. Avila, I. Razado-Colombo, C. Quaresima, C. Ottaviani, B. Olivieri, T. Bruhn, T. Hirahara, T. Shirai, S. Hasegawa, M. Carmen Asensio, G. Le Lay, *Appl. Phys. Lett.* **2013**, *102*, 163106.
- [68] P. Vogt, P. Capiod, M. Berthe, A. Resta, P. De Padova, T. Bruhn, G. Le Lay, B. Grandidier, *Appl. Phys. Lett.* **2014**, *104*, 021602.

- [69] C. Kamal, A. Chakrabarti, A. Banerjee, S. K. Deb, *J. Phys.: Condens. Matter* **2013**, *25*, 085508.
- [70] J.-L. Shi, Y. Wang, X.-J. Zhao, Y.-Z. Zhang, S. Yuan, S.-H. Wei, D.-B. Zhang, *Phys. Chem. Chem. Phys.* **2020**, *22*, 11567.
- [71] P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. Buongiorno Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carnimeo, A. Dal Corso, S. de Gironcoli, P. Delugas, R. A. DiStasio, A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gomi, J. Jia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. Küçükbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N. L. Nguyen, H.-V. Nguyen, A. Otero-de-la-Roza, L. Paulatto, S. Poncè, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu, S. Baroni, *J. Phys.: Condens. Matter* **2017**, *29*(46), 465901.
- [72] G. F. Bertsch, J.-I. Iwata, A. Rubio, K. Yabana, *Phys. Rev. B* **2000**, *62*, 7998.
- [73] <https://github.com/sheyua/RT-tddft>.
- [74] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **1996**, *77*, 3865.
- [75] J. Crank, P. Nicolson, *Adv. Comput. Math.* **1996**, *6*, 207.
- [76] T. Kopp, J. Mannhart, *J. Appl. Phys.* **2009**, *106*, 064504.

How to cite this article: Mokkath JH. Subfemtosecond charge dynamics in vertically stacked bilayer silicene. *Int J Quantum Chem.* 2021; 121:e26521. <https://doi.org/10.1002/qua.26521>

