Understanding disorder in 2D materials: the case of carbon doping of Silicene

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We investigate the effect of lattice disorder and local correlation effects in finite and periodic silicene structures caused by doping with carbon atoms using first-principles calculations. For both finite and periodic silicene structures, we show that the electronic properties of carbon-doped silicene structures are dramatically changed by controlling only one parameter, the position of substitution of carbon atoms in the structures which is related to the amount of disorder introduced in the lattice and electron-electron correlation effects. For silicene nanoclusters, the disorder is long-range due to finite-size effects while for periodic structure the disorder is short-range due to the confinement effect. By changing the position of the carbon dopants, we found that the Mott and Anderson insulators can be continuously connected as shown by the local density of states. Moreover, the bandgap is determined by the level of lattice disorder and electronic correlation effects. Finally, these structures are ferromagnetic even under disorder which has potential applications in Si-based nanoelectronics, such as field-effect transistors (FETs).

From the large variety of two-dimensional materials that exist today, silicene, the silicon counterpart of graphene has steadily increased its sphere of influence due to its malleable electronic properties and its compatibility with the current silicon-based technology.[1] Among the virtues of silicene we find i) a buckled layer geometry that facilitates band engineering and that in the presence of an electric field opens a gap transport that makes possible the realization of a field-effect transistor (FET) at room temperature;[2] ii) a stronger spin-orbit coupling than graphene that may lead to the realization of quantum spin Hall effect (QSHE) in experimentally accessible temperatures.[3] Synthesis of silicene is achieved nowadays by surface-assisted epitaxial growth on different substrates;[4-6] however, during this process, the formation of defects on the layer is practically unavoidable, which strongly influences the magnetic and electronic properties of the material.[7-11] Among the variety of possible defects, point defects can arise as a consequence of entropy maximization and thus are thermodynamically favored at high temperatures.[12, 13] Although dopants are not required by thermodynamics, they can be used as a way to control the shift of the Fermi energy. [14, 15] One-dimensional defects such as dislocations or grain boundaries arise as a consequence of imperfections in the synthetic environment or due to structural constraints imposed by the substrate.[13]

From all types of defects present in 2D materials, dopants are the most well-studied because they can potentially harness the feasibility of the electronic properties of 2D materials beyond electrically-controlled means.[14, 15] Consider, for instance, the case of phosphorus-doped silicon, a particularly well-studied example of a system showing a metal-insulator transition (MIT).[16] To create phosphorus-doped silicon, one starts with pure silicon, which is an insulator at T=0, and upon phosphorus doping, extra electrons with small ionization energy are brought into the system. Although T = 0 is necessary for this transition, several physical systems have shown an MIT at finite temperature. [17–19] Hence the importance of studying this transition. According to Mott’s argument, further increasing this dopant concentration, a transition from an insulator to metal occurs at a critical concentration, nc.[20] This transition is mediated by electronic correlation, and the concomitant lattice disorder introduced by the dopant atoms.[21, 22] An MIT which is driven mostly by the electronic correlation factor is known as Mott or Mott-Hubbard transition;[23] while an Anderson transition is driven mostly by lattice disorder.[24]

Apart from an evident theoretical interest in the Mott-Hubbard and Anderson transitions, remarkable
The semimetallic character of silicene limits its potential as a suitable material for distinct applications; however, this limitation could be overcome by the induction of Mott-Hubbard or Anderson transitions. Different authors have studied in detail silicene-graphene hybrid layers and their properties;[31, 32], however, to the best of our knowledge, there is no a systematic study on the behavior of carbon-doping in silicene in simulations or experiments. In this work, we study the doping behavior of both finite and periodic structures of silicene with carbon atoms. We have focused on carbon doping to study disorder effects and local correlations due to interactions between carbon and silicon atoms. For the sake of comparison, we have also included monovacancies in our nanoclusters. Furthermore, we compare the electronic and structural properties of periodic and finite-size structures to have a better understanding of the influence of dopant atoms on the nanoclusters.

**AB Initio Characterization.** For finite-size structures, we choose the pairing Beck 3-Parameter (exchange), Lee, Yang and Parr (B3LYP) functional with the correlation consistent polarized valence double-\(\zeta\) (cc-pVDZ) base along with D3 dispersion correction, [33] as implemented in Q-Chem 5.0. [34] For the periodic structures, the numerical simulations were carried out using plane-wave basis as implemented in the Vienna *ab initio* simulation package (VASP) code. [35–39] The exchange-correlation potential is approximated by the generalized gradient approximation (GGA) proposed by Perdew-Burke-Ernzerhof (PBE). [40] The projector-augmented wave (PAW) method is used to describe the electron-ion potential. [41] The semi-empirical Grimme-D3 dispersion corrections were also added in the present calculations in order to incorporate van der Waals dispersion effects on the system, within the default VASP parameters. [33]

**Results and discussions.** Firstly, we study the geometrical and electronic properties of a finite C-doped rectangular silicene nanocluster as shown in Fig. 1. The undoped SiNC is built from low-buckled silicene with their edges terminated by monohydrogen which is denoted by H-SiNC(4,6) and illustrated in Fig. 1a. Then, we select fourteen unequivalent doping positions \(S_1-S_{14}\) for a single C atom to substitute for a Si atom. In order to study the relative stabilities of the doped systems, the defect formation energy \(E_f\) per dopant is calculated using the following equation

\[
E_f = E_d - E_{ud} + nE_{Si} - nE_C
\]

where \(n\) is the number of dopants, \(E_d, E_{ud}, E_{Si},\) and \(E_C\) represent the total energy of doped silicene, energy of the undoped silicene, energy of a single silicon atom, and energy of a single carbon atom, respectively.

All the calculated formation energies for a single carbon substitution are listed in Table I for the singlet (an-
and triplet states at two different site positions. For the Fig. 2 the spatial spin density distribution for a singlet
netism is required for spin-based electronics, [44, 45] par-
disorder. This is an advantage since an intrinsic mag-
site and have less disorder. Furthermore, all the doped
away from the center become more stable because they
elastic in nature. In addition, we notice that all positions
the C substitutionsite because most of the distortions are
it can be seen such distortions can spread far away from
C-doping comparing with single C-doping, we com-
SiNCs are stable. However, to check the stability of dou-
C-doped H-SiNCs (4,6), the formation energies are favor-
formation energies for these configurations are listed in
S
upper (lower) edge and a total null magnetic moment indi-
cating that at this position the C atom does not have a
strong effect in the spin density compared with the
undoped H-SiNC [47]. In the triplet state, the silicene
nanocluster now exhibits a total magnetic moment since
the spin are paired-up at in opposite edges. With one C
atom at the edge (position S13) for the singlet state, the
spin density on the doped edge is locally concentrated.
It is interesting to notice that such spin density modi-
fication effect is also found in the other inner substitution
 configurations but it is gradually weakened as the C atom
is closer to the center of the nanocluster.
Now, we focus on the effect of having two carbon sub-
itations in H-SiNC(4,6). To measure the electronic cor-
relation effects between the two carbon atoms, we fix
one carbon atom at position S12 and let the other car-
substitution to be any other. We chose S12 po-
tion since it is the most stable configuration. All the
formation energies for these configurations are listed in
Table II for singlet and triplet states. As for one single
C-doped H-SiNCs(4,6), the formation energies are favor-
able (negative) which confirm that double C-doped H-
SiNCs are stable. However, to check the stability of dou-
ble C-doping comparing with single C-doping, we com-
positions can be stable for both
singlet and triplet state configurations. The tendency in

Table I. The formation energies (in eV per impurity atom) of a single C substitution at thirteen different sites of H-SiNC (4,6) for singlet (S) and triplet (T) states. All formation energies were calculated with respect to the singlet undoped ground state of H-SiNC(4,6).

| Site   | 1-Carbon (S) | 1-Carbon (T) |
|--------|--------------|--------------|
| 1      | −2.266       | −2.421       |
| 2      | −2.331       | −2.468       |
| 3      | −2.456       | −2.585       |
| 4      | −2.271       | −2.422       |
| 5      | −2.294       | −2.431       |
| 6      | −2.327       | −2.498       |
| 7      | −2.526       | −2.660       |
| 8      | −2.468       | −2.607       |
| 9      | −2.600       | −2.748       |
| 10     | −2.532       | −2.681       |
| 11     | −2.474       | −2.614       |
| 12     | −3.372       | −3.495       |
| 13     | −3.233       | −3.353       |
| 14     | −2.849       | −2.997       |

To illustrate the ferromagnetic behaviour, we show in
Fig. 2 the spatial spin density distribution for a singlet
and triplet states at two different site positions. For the
Si configuration the singlet state, the silicene nanoclus-
ter exhibits a negative (positive) magnetic moment at the

![Figure 2](image.png)
Table II. The formation energies (in eV per impurity atom) of double C substitution at thirteen different sites of H-SiNC (4,6) for singlet and triplet states. All formation energies were calculated with respect to the singlet undoped ground state of H-SiNC(4,6).

| Site | 2-C (S) | 2-C (T) | 1+1 C(S) | 1+1 (T) |
|------|---------|---------|----------|---------|
| 1    | -5.710  | -5.849  | -5.638   | -5.793  |
| 2    | -5.752  | -5.890  | -5.703   | -5.840  |
| 3    | -6.177  | -6.350  | -5.830   | -5.957  |
| 4    | -5.651  | -5.839  | -5.643   | -5.794  |
| 5    | -5.655  | -5.831  | -5.666   | -5.803  |
| 6    | -5.634  | -5.770  | -5.699   | -5.870  |
| 7    | -5.865  | -6.040  | -5.898   | -6.032  |
| 8    | -5.997  | -6.147  | -5.840   | -5.979  |
| 9    | -5.823  | -6.017  | -5.972   | -6.120  |
| 10   | -5.805  | -5.943  | -5.904   | -6.053  |
| 11   | —       | -5.952  | -5.846   | -5.986  |
| 12   | Fixed   | Fixed   | Fixed    | Fixed   |
| 13   | -6.592  | -6.690  | -6.605   | -6.725  |
| 14   | -6.242  | -6.360  | -6.221   | -6.492  |

The formation energies increase as we move from the center of the silicene nanocluster, similar to the single C doping case. For $S_{12} - S_{14}$ interaction, we need to renormalize Eq. 1 by including a carbon-carbon interaction term. Similarly, Coulomb interactions are calculated between atoms pairs. However, the Coulomb interactions are zero due to the zero partial charges at atoms of the silicene nanocluster. The results show that the two carbon atoms prefer to be apart instead of being together to form a C-C bond which would be shorter and would introduce a high strain into the structure which is more unstable compared to the silicon-silicon bond.

**Band gap analysis.** To show the effect of disorder in a H-SiNC (4,6) caused by C doping, we show in Fig. 3 the HOMO-LUMO gap for all fourteen configurations. We observed that the HOMO-LUMO gap depends on the position site and the number of C atoms in the silicene nanocluster. Here, the HOMO-LUMO gap is due to quantum confinement effects which can gap out the Dirac nodes and convert the Dirac semimetallic silicene to a band insulator. In Fig. 3a), we show the HOMO-LUMO gap for a single and double C substitution in the singlet state configuration. As it can be seen, double C doping has stronger effects in the HOMO-LUMO gap compared with single substitution. For instance, the $S_{14}$ position has a similar gap with respect to the undoped H-SiNC(4,6) with a gap of 0.467 eV. Contrary to double C substitution where the HOMO-LUMO gap is significant larger than 0.467 eV. In this case, the correlation effect is strong enough to increase the gap. As we move from position 12 (fixed position for double substitution), correlation effects and disorder decrease to be able to change significantly the HOMO-LUMO gap. Results for the triplet state are illustrated in Fig. 3b. It can be observed that the behavior in single and double C doping follows a similar trend to the singlet state. However, the effect of correlation and disorder are less effective.

**Silicene nanocluster with a dislocation and a point defect.** Since dislocations can arise as consequence of imperfections during synthesis or stress imposed through thermal history, we calculate the formation energy for a dislocation at position $S_i$ (Fig. 4a). In this case the formation energy for the dislocation is 5.082 (5.021) eV for a singlet (triplet) state configuration, which is higher than adding one C atom in the structure. Furthermore, the gap for this structure is 0.562 (0.558) eV for a singlet (triplet) state configuration, which is higher compared to the ground state H-SiNC (0.467 eV). In Fig. 4b, we simply remove one silicon atom at position $S_{i}$ from the undoped structure (Fig. 1a) and let the structure relax. This structure has a formation energy of 5.57 eV and a gap of 0.405 eV. From Fig. 4b, we can conclude that vacancies are not very stable compared to doping these silicene nanoclusters.

**Strain.** Substituting carbon atoms by Si atoms adds uniaxial strain effects on the structures which is important because the latter might be grown on a substrate with a different lattice constraint. In all cases, the unstrained relaxed structures are first obtained and then the relaxed structures are distorted by the C-doped effects. The strain is given by

$$\bar{\epsilon} = \frac{1}{3} \sum_{i=1}^{3} \frac{a_i - a_i^0}{a_i^0} \epsilon_i$$

where $a_i^0$ ($a_i$) is the equilibrium (strained) bond and $i$ represents the nearest neighbors to each carbon atom in
the doped structure. Here we only report the average strain effects on the nearest neighbor around each C atom in Table III. This consideration is used because the larger lattice distortions can be well seen at the vicinity of the C substitution, some bonds are stretched and some are compressed which can also be seen clearly in Fig. 1b and 1c. More details about the strain effect induced by the C substitution can be found in the supplemental information. Away from the C substitution, the distortions become smaller but can extend to large distance from the center of the C substitution, particularly for the positions 1, 2 and 4. Average strain follows a similar trend to the energy. The higher strain the lower the energy in the silicene nanocluster in the need to enlarge all the bonds to approximate the Si-Si bond length (2.248 Å) is longer than for for C-C bond length (1.414 Å). It seems that in order to accommodate the compressive epitaxial strain, a relatively large buckling as compared of that of freestanding silicene is induced while the Si bond lengths are maintained to similar value.

Now we turn our attention to periodic structures of silicene. For constructing the doped system, the Si atoms of the buckled (0.482 Å) structure are substitute by C atoms as in the case of silicene nanoclusters, see Fig. 5. Here, we have considered three different supercells $2 \times 2$, $3 \times 3$, and $4 \times 4$. Structures are optimized by minimizing the forces on individual atoms below 0.001 eV Å$^{-1}$ and the convergence self-consistent energy of every electron step is less than $10^{-5}$ eV. In addition, in order to avoid inter-layer interactions and simulate proper boundary conditions, a inter-layer vacuum of 10 Å below and above the each layer was added. To explore the disorder effects in these periodic structures caused by doping, we compute the formation energy as well. For a single C substitution, the formation energies are $-1.40082$ eV, $-1.5273$ eV, and $-1.6006$ eV for $2 \times 2$, $3 \times 3$, and $4 \times 4$ supercells, respectively. The negative energies indicate that doping a monolayer of silicene is energetically favourable, in agreement with the results for silicene nanoclusters.

For double C substitution, the formation energies are reported in Table IV. Positions $S_{12}$ and $S_{13}$ are not considered here due to size constrains of the lattice. According to these results, the formation energy follows the same trend as for the case of C doped silicene nanoclusters. Moreover, we can observe that position 8 is the most stable one in the $2 \times 2$ and $4 \times 4$ supercells. This shows us that the two carbons atoms prefer to be in a next nearest neighbour configuration. For periodic calculations, the distortions caused by doping are local compared with the finite size nanoclusters.

Electronic structures evolution under different site doping. The band structures of pristine silicene, double doped systems, and silicene with a monovacancy (MV) are shown in Fig. 6 alongside their respective projected density of states (DOS). In the following discussion, $S_1$ represents the only single doped system while the rest of the mentioned positions stand for a double doped system with position $S_1$ fixed. For pristine Silicene, the $\pi$ and

### Table III. The average strain effect for all thirteen positions for a single C substitution. The singlet and triplet configurations are represented by $S = 0$ and $S = 1$, respectively.

| Site | $\bar{\tau}$ (S=0) | $\bar{\tau}$ (S=1) |
|------|-----------------|-----------------|
| 1    | -0.1753         | -0.1758         |
| 2    | -0.175          | -0.175          |
| 3    | -0.1820         | -0.182          |
| 4    | -0.1761         | -0.176          |
| 5    | -0.1760         | -0.176          |
| 6    | -0.1765         | -0.176          |
| 7    | -0.1780         | -0.1785         |
| 8    | -0.1790         | -0.1784         |
| 9    | -0.1840         | -0.183          |
| 10   | -0.1810         | -0.181          |
| 11   | -0.1780         | -0.178          |
| 12   | -0.2230         | -0.223          |
| 13   | -0.1990         | -0.200          |
| 14   | -0.1970         | -0.1967         |
Figure 6. The energy band structures and Density of States (DOS) of periodic silicene with different doping positions. The last figure correspond to the Mono Vacancy (MV) case. The band structure was calculated along the path of the high symmetry points $\Gamma - K - M - \Gamma$. The blue and red lines represent the conduction (LUMO) and valence (HOMO) bands respectively. The zero in the energy axis is set at the Fermi level as shown by the dashed green line.

Table IV. Formation energies, $E_f$, and Band gaps, $E_g$, of double C substitution for spin-polarized systems at the PBE level of calculation. Here we use three different supercells. One C atom was fixed at position 1.

| Site | $2 \times 2$ | $3 \times 3$ | $4 \times 4$ |
|------|--------------|--------------|--------------|
|      | $E_f$(eV)    | $E_f$(eV)    | $E_f$(eV)    | $E_f$(eV)    | $E_f$(eV)    |
| 1    | $-1.4080$ 0.181 [I] | $-1.5273$ 0.000 | $-1.6006$ 0.099 |
| 3    | $-3.5894$ 1.006 [I] | $-3.1141$ 0.142 | $-3.1617$ 0.182 |
| 4    | $-2.1301$ 0.199 [D] | $-2.2512$ 0.041 | $-2.3306$ 0.013 |
| 6    |              | $-2.9073$ 0.050 | $-3.0507$ 0.023 |
| 7    |              | $-3.7778$ 0.000 | $-3.5401$ 0.180 |
| 8    | $-4.3472$ 0.001 [D] | $-3.7350$ 0.050 | $-3.6300$ 0.038 |
| 9    |              |              | $-3.0961$ 0.187 |
| 10   |              |              | $-3.4937$ 0.034 |
| 11   |              |              | $-3.5396$ 0.183 |
| MV   | 2.9956 0.458 [D] | 3.2189 0.003 | 3.2918 0.074 |

$\pi^*$ bands cross linearly at the Fermi Level ($E_F$) at the symmetric $K$ point in the reciprocal space, forming the so-called “Dirac cones”. In the vicinity of these points, the energy-momentum dispersion varies linearly near the Fermi energy. We can immediately recognize the zero band gap of pristine Silicene; however, unlike Graphene, the low-buckled structure of Silicene grants it an easily tunable band-gap.

When we doped Silicene with one carbon atom, the symmetry between the sublattices is broken, this results in a moderate indirect bandgap (in the K and G points) of 0.181 eV with a semiconductor behavior. Depending on the sublattice position, adding an additional carbon atom could break the symmetry of the system, even more, resulting and large bandgap; this is the case for the C3 system (same sublattice) which shows an indirect gap of 1.006 eV and semiconductor behavior. On the other hand, the systems C4 and C8 act on different sublattices and show bandgaps of 199 and 1 meV respectively. Both systems present a direct gap; yet, the C4 gap is around the G point and C8 in the K direction. For these two last systems, C4 induces the most distortion in the lattice as its C-Si and Si-Si are 0.157 and 0.139 Å longer than those in C8 (comparison is made for the nearest neighbor atoms). Another remarkable difference is that the C4 system is a semiconductor while C8 a semimetal. Therefore, we observed a band splitting proportional to the amount of disorder and local interactions between the lower and the upper bands as shown by the density of states in Fig. 6.

Thus the position doping dependence is related to the amount of disorder and electronic interactions induced by the carbon atoms. This indicates that the Mott and Anderson insulators are continuously connected. Hence, by changing the position of carbon atoms, it is possible to tune the electronic correlations and disorder and move from one type of insulator to the other without crossing the semimetallic phase. This is possible because the Anderson transition (no electron correlation) is not associated with symmetry breaking. [21] These results are in agreement with the finite silicene nanoclusters. The electronic structure of the 2x2 MV indicates a metallic behavior, with a sizeable direct bandgap of 0.458 eV. We do not observe self-healing for any of the MV systems, although, for the 4x4 system, there seems to be a slight
tendency towards it, as two of the silicene atoms in the deficiency approach each other at a distance of 2.64 Å. More importantly, when the defect’s concentration is diluted, we observe a transition from a metal to a semimetal going from the 2x2 to the 3x3 system; another transition occurs from a semimetal to semiconductor going from the 3x3 to 4x4 system. This concentration-dependent transition has been previously reported in silicene for other periodicities. In particular, Yang et al. found metal to semiconductor transitions in their study. [48]

In conclusion, using first-principles calculations, we study the effects of disorder on the electronic properties of silicene nanocluster caused by C doping. Total energies analysis indicates that C tends to be doped at the edges of finite silicene structures, which are ferromagnetic. For these finite structures, the bandgap depends strongly on the effect of disorder and correlation effects, which is related to the Anderson-Hubbard model for arbitrary interaction and disorder. Besides, for finite structures is more feasible to do chemical doping than having dislocations. For periodic structure, the electronic properties also change depending on the amount of disorder and correlation effects caused by the carbon atoms. When there is no enough disorder and weak correlation, the electronic dispersion is characterized by Dirac cones at $K$ and $K'$ directions, while the conduction bands split into two different modes from the $M - G$ direction. As the disorder and strong correlation are present, the Dirac cones do not longer exist, or they move away from the $K$ points. This indicates that the Mott and Anderson insulators are continuously connected. The specific predictions of our simulations not only apply to silicene but also other doped 2D materials. [49] Moreover, it is anticipated that these theoretical results may be valuable in the design of Silicene-based electronic devices with control over the spins in spintronics. [44, 45]

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[1] Jijun Zhao, Hongsheng Liu, Zhiming Yu, Ruge Qhe, Si Zhou, Yangyang Wang, Cheng Cheng Liu, Hongxia Zhong, Nannan Han, Jing Lu, Yugui Yao, and Kehui Wu, “Rise of silicene: A competitive 2d material,” Progress in Materials Science 83, 24 – 151 (2016).
[2] Zeyuan Ni, QiQiang Liu, KeChao Tang, Jiaxin Zheng, Jing Zhou, Rui Qin, Zhengxiang Gao, Dapeng Yu, and Jing Lu, “Tunable bandgap in silicene and germanene,” Nano Letters 12, 113–118 (2012), pMID: 22050667, https://doi.org/10.1021/nl203065e.
[3] Cheng-Cheng Liu, Wanxiang Feng, and Yuguí Yao, “Quantum spin hall effect in silicene and two-dimensional germanium,” Phys. Rev. Lett. 107, 076802 (2011).
[4] Boubekeur Lalmi, Hamid Oughaddou, Hanna Enriquez, Abdelkader Kara, Sébastien Vizzini, Bénédicte Ealét, and Bernard Aufray, “Epitaxial growth of a silicene sheet,” Applied Physics Letters 97, 223109 (2010), https://doi.org/10.1063/1.3524215.
[5] Lei Meng, Yeliang Wang, Lizhi Zhang, Shizuan Du, Rongtian Wu, Linfei Li, Yi Zhang, Geng Li, Haitao Zhou, Werner A. Hofer, and Hong-Jun Gao, “Buckled silicene formation on ir(111),” Nano Letters 13, 685–690 (2013), pMID: 2333062, https://doi.org/10.1021/nl304347w.
[6] Antoine Fluereonce, Rainer Friedlein, Taisuke Ozaki, Hirokuni Kawai, Ying Wang, and Yukiko Yamada-Takamura, “Experimental evidence for epitaxial silicene on diboride thin films,” Phys. Rev. Lett. 108, 245501 (2012).
[7] Gian G Guzmán-Verri and LC Lew Yan Voon, “Electronic structure of silicon-based nanostructures,” Physical Review B 76, 075131 (2007).
[8] Seymour Cahangirov, Mehmet Topsakal, Ethem Aktürk, H Şahin, and Salim Ciraci, “Two-and one-dimensional honeycomb structures of silicon and germanium,” Physical review letters 102, 236804 (2009).
[9] Abdelkader Kara, Hanna Enriquez, Ari P. Seitsonen, LC Lew Yan Voon, Sébastien Vizzini, Bernard Aufray, and Hamid Oughaddou, “A review on silicene—new candidate for electronics,” Surface science reports 67, 1–18 (2012).
[10] Zhong Lin, Bruno R Carvalho, Ethan Kahn, Ruitao Lv, Rahul Rao, Humberto Terrones, Marcos A Pimenta, and Mauricio Terrones, “Defect engineering of two-dimensional transition metal dichalcogenides,” 2D Materials 3, 022002 (2016).
[11] S Li, Yifeng Wu, Yi Tu, Yonghui Wang, Tong Jiang, W Liu, and Yonghao Zhao, “Defects in silicene: Vacancy clusters, extended line defects, and di-adatoms,” Scientific Reports 5, 7881 (2015).
[12] Junfeng Gao, Junfeng Zhang, Hongsheng Liu, Qinfang Zhang, and Jijun Zhao, “Structures, mobilities, electronic and magnetic properties of point defects in silicene,” Nanoscale 5, 9785–9792 (2013).
[13] Shuang Li, Yifeng Wu, Yi Tu, Yonghui Wang, Tong Jiang, Wei Liu, and Yonghao Zhao, “Defects in silicene: vacancy clusters, extended line defects, and di-adatoms,” Scientific reports 5, 7881 (2015).
[14] J-H Chen, Ci Jiang, S Adam, MS Fuhrer, ED Williams,
and Masa Ishigami, “Charged-impurity scattering in graphene,” Nature Physics 4, 377 (2008).
[15] B Sachs, L Britnell, TO Wehling, A Eckmann, R Jalil, BD Belle, AI Lichtenstein, MI Katsnelson, and KS Novoselov, “Doping mechanisms in graphene-mos2 hybrids,” Applied Physics Letters 103, 251607 (2013).
[16] T. F. Rosenbaum, R. F. Milligan, M. A. Paalanen, G. A. Thomas, R. N. Bhatt, and W. Lin, “Metal-insulator transition in a doped semiconductor,” Phys. Rev. B 27, 7509–7523 (1983).
[17] S Anissimova, SV Kravchenko, A Punnoose, MP Lilly, JL Reno, JA Simmons, IB Spielman, JP Eisen-...
nanoclusters,” Physical Review Applied 9, 054012 (2018).

[48] Muhammad Ali, Xiaodong Pi, Yong Liu, and Deren Yang, “Electronic and magnetic properties of graphene, silicene and germanene with varying vacancy concentration,” AIP Advances 7, 045308 (2017), https://doi.org/10.1063/1.4980836.

[49] D Usachov, O Vilkov, A Gruneis, D Haberer, A Fedorov, VK Adamchuk, AB Preobrajenski, P Dudin, A Barinov, M Oehzelt, et al., “Nitrogen-doped graphene: efficient growth, structure, and electronic properties,” Nano letters 11, 5401–5407 (2011).