Graphene's morphology and electronic properties from discrete differential geometry

Alejandro A. Pacheco Sanjuan,1 Zhengfei Wang,2 Hamed Pour Imani,3 Mihajlo Vanević,4 and Salvador Barraza-Lopez3
1. Departamento de Ingeniería Mecánica. Universidad del Norte. Km. 5 Vía Puerto Colombia. Barranquilla, Colombia
2. Department of Materials Science. University of Utah. Salt Lake City, UT 84112, USA
3. Department of Physics. University of Arkansas. Fayetteville, AR 72701, USA
4. Department of Physics. University of Belgrade. 11158 Belgrade, Serbia

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The geometry of two-dimensional crystalline membranes dictates their mechanical, electronic and chemical properties. The local geometry of a surface is determined from the two invariants of the metric and the curvature tensors. Here we discuss those invariants directly from atomic positions in terms of angles, areas, vertex and normal vectors from carbon atoms on the graphene lattice, for arbitrary elastic regimes and atomic conformations, and without recourse to an effective continuum model. The geometrical analysis of graphene membranes under mechanical load is complemented with a study of the local density of states (LDOS), discrete induced gauge potentials, velocity renormalization, and non-trivial electronic effects originating from the scalar deformation potential. The asymmetric LDOS is related to sublattice-specific deformation potential differences, giving rise to the pseudomagnetic field. The results here enable the study of geometrical, mechanical and electronic properties for arbitrarily-shaped graphene membranes in experimentally-relevant regimes without recourse to differential geometry and continuum elasticity.

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Introduction.- Graphene [1, 2] belongs to a family of atom-thin elastic membranes [3] that conform to harder surfaces (e.g., [4]), develop ripples when freestanding [5–17], and can be deformed into arbitrary elastic regimes [18], leading to a remarkable electronic response [18–33]. In general, the local geometry of a two-dimensional (2D) surface is determined by four invariants of its metric (\(g\)) and curvature (\(k\)), that indicate how much it stretches and curves with respect to a reference non-deformed shape. Suitable choices are the determinant and the trace of \(g\), the Gauss curvature \(K \equiv \det(k)/\det(g)\), and the mean curvature \(H \equiv \text{Tr}(k)/2\text{Tr}(g)\) [34–36].

In the existing literature, graphene’s geometry is commonly studied in terms of a continuous displacement field \(u_\alpha(\xi^1, \xi^2)\). Specifically, on thin-plate continuum elasticity the strain tensor is

\[
g_{\alpha\beta} = \delta_{\alpha\beta} + 2u_{\alpha\beta}, \quad k_{\alpha\beta} = \hat{n} \cdot \frac{\partial g_{\alpha\beta}}{\partial \xi^\beta}, \quad (1)
\]

where \(g_{\alpha}(\xi^1, \xi^2)\) is a tangent vector field, \(\delta_{\alpha\beta}\) is the reference (flat) metric and \(\hat{n} = \frac{\mathbf{e}_1 \times \mathbf{e}_2}{|\mathbf{e}_1 \times \mathbf{e}_2|}\) is the local normal. **Strain engineering clearly is a geometrical theory** that applies to arbitrarily-shaped graphene without topological defects. Here, Wigner-Seitz unit cells are the underlying discrete geometrical objects and atomistic information is always preserved. The discrete formalism for geometry and the electronic response of Dirac fermions rests on interatomic distances without a mediating continuum. The framework here realized is non-perturbative on the geometry, and it can be used to indicate if the sublattice symmetry is preserved in the system at hand (this is assumed in the continuum theory [21]) and to show how the reciprocal space is renormalized by strain [33]. In what follows, we present the tools for geometrical analysis, study the local geometry of rippled graphene [13], and discuss the discrete geometry and the electronic properties of graphene under central load.

**The discrete geometry.**- The discrete metric is defined from the local lattice vectors \(\mathbf{a}_\alpha\) [10, 11, 14, 47], \(g_{\alpha\beta} = \mathbf{a}_\alpha \cdot \mathbf{a}_\beta\) [Fig. 1(a-b)], and the discrete Gauss curvature \((K_D)\) originates from the **angle defect** \(\sum_{i=1}^{6} \theta_i / A_p\) [44–46]:

\[
K_D = (2\pi - \sum_{i=1}^{6} \theta_i) / A_p. \quad (2)
\]

Here \(\theta_i\) \((i = 1, ..., 6)\) are angles between vertices shown in Fig. 1(a). The *Voronoi tessellation* [dark blue in Fig. 1(a)]
with an area $A_p$, generalizes the Wigner-Seitz unit cell on conformal 2D geometries. (The angle defect adds up to $2\pi$ on a flat surface, making $K_D = 0$, as expected.)

The discrete mean curvature $H_D$ measures relative orientations of edges and normal vectors along a closed path:

$$H_D = \sum_{i=1}^{6} e_i \times (\nu_{i,i+1} - \nu_{i-1,i}) \cdot \hat{n}/4A_p.$$  \hspace{1cm} (3)

Here, $v_i$ is the position of atom $i$ on sublattice $A$, and $e_i = v_i - v_p$ is the edge between points $p$ and $i$ (note that $a_{12} = e_{12}$). $\nu_{i,i+1}$ is the normal to edges $e_i$ and $e_{i+1}$ (i is a cyclic index), and $\hat{n} = \sum_{i=1}^{n} \nu_{i,i+1}/A_i$ is the area-weighted normal with $A_i = |e_i \times e_{i+1}|/2$ [44]. For the purposes of discrete geometry, the metric and curvatures are normally decoupled objects.

The discrete metric and curvatures furnish geometry consistent with a crystalline structure, and lead to the faithful characterization of graphene’s morphology beyond the effective-continuum paradigm, Eq. (1). This is advantageous when the atomic conformation is known from molecular dynamics (e.g. [13]) or experiment (e.g., [45]) because: (i) fitting of the atomic lattice to an effective continuum is not needed any more, (ii) the Chemistry of conformal graphene can be addressed from the discrete geometry [42] and, since atoms are always available, (iii) the discrete theory brings new insights and understanding into the physical theory (e.g., non-preservation of sublattice symmetry, the form of gauge fields [10], the creation of mass from strain [11, 29]). We emphasize that the discrete geometry is accurate regardless of elastic regime, hence it can be used to verify whether the conditions for continuum elasticity hold in the problem at hand.

**Continuum geometry for small deformations.** The new framework does capture the known (continuum) geometry when the latter applies. This is illustrated in Fig. 1(c) for a profile $z(r) = A \exp[-r^2/\sigma^2]$ with $A=0.8$ Å and $\sigma=50$ Å [23]. The continuum geometric invariants are: $\det(\tilde{g}) = 1 + 4r^2z^2/\sigma^4$, $\text{Tr}(\tilde{g}) = 2 + 4r^2z^2/\sigma^4$ (both are radial-symmetric), $K = \frac{z''}{1+z^2z''''}$, and $\tilde{H} = \frac{4z''}{2+4z^2z'''} + \frac{z'''}{1+z^2z''''}$. We next lay out a crystalline graphene lattice with discrete coordinates $(x_i, y_i, 0)$, and assign $z_i \equiv z(r_i)$ to each atom, with $r_i = \sqrt{x_i^2 + y_i^2}$. For easy comparison with the continuum metric, we renormalize $g$ with respect to the flat discrete metric $(z_i = 0)$ $[\det(g_{00}) = 3\alpha^4/4$, and $\text{Tr}(g_{00})/2 = \alpha^2]$, and plot $1-\text{det}(\tilde{g})$ and $2-\text{Tr}(g)$ to emphasize deviations from the reference metric. $\Delta \sqrt{\det(g)} = \sqrt{\det(\tilde{g})} - \sqrt{\det(g)}$ and $\Delta \text{Tr}(g) = \text{Tr}(\tilde{g}) - \text{Tr}(g)$ in Fig. 1(c) point to small discrepancies among the discrete (g) and continuum ($\tilde{g}$) [33, 35] metrics, originating already because $\tilde{g}$ is built from tangent vector fields $\tilde{g}_{ij}$ as two points along a continuum geodesic collapse onto each other, and this limiting process does not take place on the atomic lattice [see Fig. 1(b)]. Those discrepancies aggravate under extreme morphologies for which the discrete geometry lacks smooth approximations in between atomic positions. On the other hand, $K_D = K$ and $H_D = H$ [Fig. 1(e)], highlighting the meaning of curvature from atoms [Eqs. (2-3)].

To make the discrete $(g)$ and continuum $(\tilde{g})$ metrics correspond with one another, $\tilde{g}$ must be corrected at atomic positions as follows: $g_{\alpha\beta} = b_{\alpha}^i b_{\beta}^j g_{ij} + b_{\alpha}^i b_{\beta}^j$, where $g_{ij} = \tilde{g}_i \times \tilde{g}_j / |\tilde{g}_i \times \tilde{g}_j|$ and $b_{\alpha}^k = a_{\alpha}^i g_{ki}$ ($\alpha, \beta = 1, 2, i, j, k = 1, 2, 3$). The first term accounts for the anisotropy of the honeycomb lattice, while the second one is an exponential map that brings continuum tangent fields $\tilde{g}_i$ back onto the atomistic surface [33, 34, 35].

**Rippled graphene.** The importance of a sound geometrical framework is motivated by rippled graphene. We contrast ripples created by thermal fluctuations [13] with those created at low temperature due to edges. These two mechanisms lead to different types of geometries (hence different magnitudes of strain-derived gauges). In a system with periodic boundary conditions, thermal fluctuations create significant changes in interatomic distances (i.e., in the metric) [13] and as the boundaries are fixed—such increases on interatomic distances reflect on out-of-plane deformations (i.e., rippling).

Now consider a square graphene sample with about three million atoms, and relieve strain at the edges at the low temperature of 1 Kelvin. The resulting membrane is shown in Fig. 2(a), where colors indicate varying heights across the sample [11]. Ripples in Ref. [13] originate from increases in the metric. On the other hand, the white margin in between the “rippled” (curved) sample and the (yellow) exterior frame highlights an apparent contraction of our finite sample when seen from above.

The details of this geometry are shown in Fig. 2(b).
We find that det$(g)$ and $\text{Tr}(g)$ are unity almost everywhere (yet there are significant random fluctuations driving the scales): The metric tells us that the membrane does not contract and its area thus remains almost unchanged. We show in Fig. 2(b) the discrete curvatures, highlighting cusps by ovals, valleys by squares, and ridges by triangles. Cusps and valleys have the largest Gauss curvature $K_D$ (deep red), while ridges have the smallest one (deep blue). As expected, the mean curvature $H_D$ takes its largest (smallest) value at valleys (cusps) and alternates sign around ridges. The curvature without metric increases explains the white margins on Fig. 2(a).

The discrete geometry reflects the mechanism leading to ripple formation: This highlights the virtues of a geometry originating from atoms. In particular, an accurate determination of $H_D$ is important since $H_D$ leads to spin diffusion in rippled graphene [41, 50, 51]. Though much has been said about ripples, no geometrical study with the accuracy and insight provided here exists. The geometrical invariants in Fig. 2(b) are larger in magnitude than those in Fig. 1(c) – obtained by a smooth deformation from the reference ($z = 0$) initial configuration.

The starting point in the continuum theory is a flat metric $\delta_{\alpha\beta}$. There, a non-zero curvature directly leads to increases in interatomic distances [Eq. (1)], and a non-zero height is directly identified with a non-zero strain-derived gauge. A question then arises whether the sample under study actually obeys Eq. (1). The situation shown in Fig. 2 is a counterexample to the geometry inferred from Eq. (1) because the metric is almost constant even though the height profile $z$ is clearly non-flat (for a pseudo-length-preserving distortion). Gauge fields for similar samples were reported in Ref. [11]. Rippled graphene is an excellent example that shows how crucial it is to know the exact geometry on a case-by-case basis, and Fig. 2 represents the accurate geometrical characterization of rippled graphene down to the atomic level.

**Graphene under load.** Next we analyze a circular freestanding membrane [32] created by clamping the graphene sample in Fig. 2(a) outside a radius $R = 700 \text{ Å}$ from the geometrical center. We push the membrane down to a depth $z_0$ with a spherical tip of radius $r_t = 15 \text{ Å}$ [Fig. 3(a)]. The tip has constant curvatures $K_t = 1/r_t^2 = 4.4 \times 10^{-3} \text{ Å}^{-2}$ and $H_t = 1/r_t = 0.07 \text{ Å}^{-1}$.

Figure 3(b) tells us quantitatively how graphene gradually conforms to the tip pushing it down. $g$ increases without bound (four upper plots in Fig. 3(b)) until an eventual mechanical breakdown [18]. $(\text{Tr}(g)/2)^{1/2}$ [from Fig. 3(b)] informs of large increases of interatomic distances, up to $\sim 26\%$ for loads where $z_0 = -215 \text{ Å}$, beyond the realm of first-order continuum elasticity [Eq. (1)]. The discrete metric $g$ also uncovers an asymmetric elongation between armchair (vertical) and zigzag (horizontal) directions which the continuum metric $\hat{g}$ does not capture unless corrected as indicated above.

On the other hand, graphene cannot acquire a curvature higher than that of the tip, so $K_D$ and $H_D$ must be bounded. This is precisely the content of the two lower plots in Fig. 3(b): For small loads ($z_0 = -8 \text{ Å}$; ellipses) the curvatures are almost zero as expected. Curvatures increase (star, rectangle and triangle) as the magnitude of $z_0$ increases ($z_0 = -50, -100$, and $-215 \text{ Å}$, respectively). The important observation is that curvatures saturate ($K_D \rightarrow K_t$ and $H_D \rightarrow H_t$) for distances $r$ within $r_t$ (shaded area), confirming the qualitative conformal shape depicted on Fig. 3(a). $K_D$ and $H_D$ have analogous trends in Figs. 1 and 3 [$H_D$ is a signed quantity, having opposite signs for a bulge (Fig. 1) and a sag (Fig. 3)]. Yet, it remains a challenge to accurately describe the geometry shown in Fig. 3 within the continuum formalism using Eq. (1). This is so, because for high load the metric and curvature appear decoupled, while in the continuum approach they are inexorably inter-related.

**Microscopic mass term and gauge fields.** Next, we analyze electronic properties of graphene under load by the tip. We first re-express the microscopic pseudo-magnetic field from the curl of the (pseudo-magnetic) vector potential. This is accomplished with a second-order difference...
relation among potential energies for an atom on the A-sublattice at the K-point [Fig. 4(a)]

\(- \mu_B B_s \rho = \frac{\sqrt{\delta t^2}}{m_{e}a_{B}^2} ((\delta t_3^{(3)} - \delta t_1^{(3)}) - (\delta t_3^{(2)} - \delta t_1^{(2)}) \) (4)

\(+ (\delta t_3^{(3)} - \delta t_2^{(3)}) - (\delta t_3^{(1)} - \delta t_2^{(1)}) \).

Here, \(\mu_B\) is the Bohr magneton (\(\approx 5.8 \times 10^{-5}\) eV/Tesla), \(\delta t_i^{(n)}\) is the standard change in hopping upon strain at unit cell \(n = 1, 2, 3\) \[10, 19, 21, 22\], and \(\sqrt{\delta t^2} / m_{e}a_{B}^2 \approx 2.5\) \[47\]. The pseudomagnetic field \(B_s\) changes sign at the B-sublattice and/or at the K’ point \[2, 51\]. \(E_s\) is the average deformation potential at a given unit cell (see Refs. \[10\] and \[47\]) arising from the rearrangement of the electron cloud upon strain \[19\]. \(B_s\) is shown on Fig. 4(b) for \(z_0 = -100\) and \(z_0 = -215\) within a 75 Å radius from the tip.

Local density of states.- The shaded area plots on Fig. 4(c) and Fig. 4(a-b) are reference LDOS obtained from a flat configuration with no strain. The metric and curvature in Fig. 3(b) take extreme values at \(r = 0\), and the LDOS in Fig. 4(c) increase in slope as the Fermi velocity \(v_F\) becomes more and more renormalized \[23, 25\] as \(LDOS \propto 1/v_F^2\) \[2\]. Remarkably, in the scenario given by Fig. 3(b), the metric increase enhances the velocity renormalization while, at the same time, the curvature remains the same. This is so because the observed Fermi velocity renormalization is related to \(g\): Indeed, it is caused by changes in interatomic distances \[19, 22\].

When a screened \(E_s\) is applied, \(v_F\) renormalization becomes electron-hole asymmetric \[2, 43\], and a sequence of equally-spaced peaks arise even without explicit inclusion of spin (we do not have a quartet-splitting mechanism \[32\]). Thus, our results suggest an alternative explanation for the identically-scaled LDOS features observed in a similar experimental setup \[32\] (in particular, refer to Fig. 4(c) with \(z_0 = -215\) Å, where \(E_s\) is larger). We emphasize that there is no central LDOS peak (‘zeroth Landau level’) for circular membranes under load.

The dashed LDOS curves in Fig. 5 were plotted with \(E_s = 0\), while the asymmetric LDOS profiles – displaying equally-spaced peaks – were obtained with a (screened) \(0.25 E_s\) deformation potential. On Figs. 5(a-b) we explore the LDOS in space and exclusively on the A-sublattice, generated from a \(z_0 = -100\) Å load. Figure 5(a) shows the LDOS along the \(-30^\circ\) (orange/light) and \(+30^\circ\) (brown/dark) radial axes on the polar grid in display on Figs. 5(c) and 5(d). Due to threefold symmetry, the LDOS is identical upon \(120^\circ\) rotations. \(B_s \sim 0\) in Fig. 5(a) as it alternates sign at those axes. Hence, the only observable effect is a LDOS renormalization due to the metric \[23\] \((r = 20\) Å plot). The renormalization gradually decreases with increasing \(r\) until the LDOS overlaps with the reference one (see \(r = 75\) Å plot), consistent with a metric approaching the flat one [Fig. 3(b)]. On the other hand, under a non-zero \(B_s\) the LDOS on the A-sublattice either becomes enhanced (blue curves; \(B_s < 0\); \(60^\circ\) axis) or suppressed (red; \(B_s > 0\); \(0^\circ\) axis) with respect to the reference LDOS [Fig. 5(b)]. Figure 4(a) complements previous reports \[51\].

Due to time-reversal symmetry, the A- and B-sublattices are subjected to \(B_s\) with opposite signs and the behavior on Fig. 5(b) should be reproducible by exploring the LDOS under the same \(B_s\), but now at the B-sublattice (exchanging \(K\) to \(K'\) amounts to a sublattice exchange \[15\]). This is verified on Fig. 5(c-d) by the sublattice resolved angular sweep across a \(B_s > 0\) feature. A sublattice asymmetric LDOS [Fig. 5(c-d)] is consistent with a sublattice-dependent potential, Eq. 4, through Coulomb’s law.

Conclusion.- We presented a discrete approach to study graphene’s geometry and its electron properties without relying on continuum approximations and beyond thin-plate continuum mechanics. We used the method to study the experimentally relevant situations of rippled graphene and graphene under large mechanical load. Our theory fully respects the discrete geometry of arbitrarily-shaped graphene, thus opening a completely unexplored and promising route for strain-engineering beyond the restrictions of small and slowly-varying deformations inherent to continuum theories. We thank M.A.H. Voz-
mines a proper discrete surface, and develops theory for DDG. That graphene’s lattice is made of polyhedra, it represents DDG, in turn, seeks for discrete equivalents of notions that continuous geometry studies geometrical shapes made of polyhedra.

The aims of the main manuscript are to develop mathematically sound relations between differential and discrete geometry, and to develop theories from that discrete surface. In the absence of an actual atomic lattice, one can suggest many different discretizations of surfaces having the same continuum limit. For graphene, on the other hand, the honeycomb lattice is the discrete lattice, and no more fundamental choice exists without involving approximations.

This represents a central difference between an all-discrete theory and discrete approximations of continuum models. In the latter, discretization of surfaces and differential equations is carried out on an arbitrary mesh. In the context of strain engineering in graphene, this process starts the moment the theory of an arbitrary continuum media is mapped onto arbitrary meshes for numerical analysis. In applying DDG to graphene, on the other hand, the mesh is given by the deformed honeycomb lattice, and we never take the continuum limit of the pseudospin Hamiltonian when considering the electronic behavior either. The results of DDG are therefore non-perturbative on graphene’s atomistic morphology.

Discrete geometry for substantial distortions: On page 2 of the main manuscript we demonstrate that the discrete and continuum geometries agree in the limit of small deformations; this is, when the distortion is small when compared to interatomic distances. For large deformations, the continuum hypothesis breaks down as continuum tangent fields cannot be generated to arbitrary precision from atomic locations.

To show the breakdown of the continuum geometrical description, we display in Fig. 1 the geometry for the function $z(x_0, y_0) = A[\exp\left(-\frac{(x-x_0)^2+(y-y_0)^2}{\sigma^2}\right) - \exp\left(-\frac{(x-x_0)^2+(y-y_0)^2}{\sigma^2}\right)]$, with $A = 25 \ A$, $\sigma = 30 \ \AA$, and $x_0 = 25 \ \AA$. Here, the continuum geometrical invariants display large discrepancies to the discrete geometry; this is particularly the case for the trace of the metric.

As a consequence of such discrepancies, the continuum idealization of the atomic membrane will have an inaccurate distribution, which can be incompatible with the actual lattice structure. A subcell deficiency, tangent vectors $g_{ij}$, may lie outside of the polygonal surface, compromising mechanical equilibrium. An exponential map bringing the continuum vector field back onto the atomistic surface becomes necessary, and the continuum metric $\tilde{g}_{ij}$ must be corrected at atomic positions to properly conform to $g$.

**The mean deformation potential $E_s$** - This empirical expression was introduced before (Eqn. (18) in Ref. [10]), and it has the radial shape illustrated in Fig. 1 for loads $z_0 = -100 \ \AA$, and $z_0 = -215 \ \AA$. Proper consideration of those changes on the local potential cannot be given by consideration of nearest neighbors alone, and a second-order difference equation is needed. Here we derive microscopic expressions for the pseudo-magnetic field, when the zigzag direction is parallel to the y-axis (i.e., zigzag direction parallel to x-axis and y-axis) can be obtained along similar lines.

The program of action is as follows: We wish to express the magnitude of the finite-difference pseudo-magnetic field $B_0$ as a function of local changes in the vector potential. $B_0$ will display a straightforward and physically intuitive form in terms of energy variations $\delta t$ among neighboring atoms belonging to complementary sublattices. These variations are similar in origin to the ones we reported.
where \( \tau_1 = (1/2, \sqrt{3}/2) a_0 / \sqrt{3} \), \( \tau_2 = (1/2, -\sqrt{3}/2) a_0 / \sqrt{3} \), and \( \tau_3 = (1, 0) a_0 / \sqrt{3} \). \( \delta t_j = -|\beta| |\tau_j \cdot \Delta \tau_j| / a_0^2 \), see Refs. [10, 22] for details. We choose \( \mathbf{K} = (0, 1) a_0^2 \) as well. Then:

\[
\sum_{j=1}^{3} \delta t_j^{(n)} e^{i \mathbf{K} \cdot \mathbf{r}_j} = \frac{-\sqrt{3}}{2} \left[ \frac{2\delta t_3^{(n)} - \delta t_1^{(n)} - \delta t_2^{(n)}}{\sqrt{3}} + i(\delta t_1^{(n)} - \delta t_2^{(n)}) \right].
\]

The upper index \( (n) \) enters in Eq. (8) because the discrete curl (a term arising from differences of \( \delta t \) in between sublattices) requires obtaining differences of \( \sum_{j=1}^{3} \delta t_j^{(n)} e^{i \mathbf{K} \cdot \mathbf{r}_j} \) on three adjacent unit cells Fig. 8, \( n = 1, 2, 3 \). Consistent with the choice of zigzag direction, the \( x \) and \( y \) components of the vector potential dictate the choice of components in Eq. (8). To simplify the algebra, we introduce:

\[
\begin{align*}
 f_x(A) & \equiv \delta t_2^{(2)} - \delta t_1^{(1)}, \\
f_y(A) & \equiv \frac{2\delta t_3^{(3)} - \delta t_1^{(1)} - \delta t_2^{(2)}}{\sqrt{3}}, \\
f_x(B_1) & \equiv \delta t_2^{(1)} - \delta t_1^{(1)}, \\
f_y(B_1) & \equiv \frac{2\delta t_3^{(3)} - \delta t_1^{(1)} - \delta t_2^{(2)}}{\sqrt{3}}, \\
f_x(B_2) & \equiv \delta t_2^{(2)} - \delta t_1^{(2)}, \\
f_y(B_2) & \equiv \frac{2\delta t_3^{(3)} - \delta t_1^{(2)} - \delta t_2^{(3)}}{\sqrt{3}}, \\
f_x(B_3) & \equiv \delta t_2^{(3)} - \delta t_1^{(3)}, \\
f_y(B_3) & \equiv \frac{2\delta t_3^{(3)} - \delta t_1^{(2)} - \delta t_2^{(3)}}{\sqrt{3}}.
\end{align*}
\]

We use Eq. (8) to establish the discrete local curl in terms of differences of function \( f = (f_x, f_y) \) at neighboring positions corresponding to complementary sublattices:

\[
\nabla \times \mathbf{f} \equiv (\Delta_x f_y - \Delta_y f_x) \mathbf{n}.
\]

Then, finite-differences become:

\[
\Delta_x f_y = \frac{f_x(A) - f_x(B_3)}{(\tau_3 + \Delta \tau_3)} \mathbf{i} + \frac{f_x(A) - f_x(B_2)}{(\tau_2 + \Delta \tau_2)} \mathbf{i} + \frac{f_x(A) - f_x(B_1)}{(\tau_1 + \Delta \tau_1)} \mathbf{i},
\]

and:

\[
\Delta_y f_x = \frac{f_y(A) - f_y(B_2)}{(\tau_2 + \Delta \tau_2)} \mathbf{j} + \frac{f_y(A) - f_y(B_1)}{(\tau_1 + \Delta \tau_1)} \mathbf{j}.
\]
\(\hat{i}\) and \(\hat{j}\) represent local in-plane vector fields:

\[
\hat{i} = \frac{a_1 + a_2}{|a_1 + a_2|}, \quad \hat{j} = \frac{a_1 - a_2}{|a_1 - a_2|},
\]

with \(a_1 = \tau_1 + \Delta \tau^{(3)}_1 - (\tau_3 + \Delta \tau^{(3)}_3)\) and \(a_2 = \tau_2 + \Delta \tau^{(2)}_2 - (\tau_3 + \Delta \tau^{(3)}_3)\) the local lattice displacements for a central atom on the \(A\) sublattice, and \(n\) was defined in Eq. 2 in the main text. Using Eq. (9), we get for Eqs. (11) and (12):

\[
\Delta_x f_y = \frac{(\delta t^{(1)}_1 + \delta t^{(2)}_1) - (\delta t^{(1)}_1 + \delta t^{(2)}_2)}{(\tau_3 + \Delta \tau^{(3)}_3) \cdot \hat{i}} + \frac{2\delta t^{(3)}_3 - \delta t^{(1)}_1 - (2\delta t^{(2)}_3 - \delta^{(2)}_2)}{2\delta t^{(3)}_3 - \delta t^{(1)}_2 - (2\delta t^{(2)}_3 - \delta^{(2)}_1)} + \frac{2\delta t^{(3)}_3 - \delta t^{(1)}_2 - (2\delta t^{(2)}_3 - \delta^{(2)}_1)}{(\tau_1 + \Delta \tau^{(3)}_1) \cdot \hat{i}},
\]

and:

\[
\Delta_y f_x = \frac{\delta t^{(2)}_1 - \delta t^{(1)}_1}{(\tau_2 + \Delta \tau^{(2)}_2) \cdot \hat{j}} + \frac{\delta t^{(2)}_2 - \delta t^{(1)}_2}{(\tau_1 + \Delta \tau^{(3)}_1) \cdot \hat{j}}.
\]

Next, we require hermiticity of a vector potential (these conditions are not needed for a scalar potential term, which is Hermitian by construction). The conditions are (see [21] and [10][11] for extended discussion):

\[
\tau_1 + \Delta \tau^{(1)}_1 \rightarrow \tau_1 + \Delta \tau^{(3)}_1, \quad \text{and} \quad \tau_2 + \Delta \tau^{(2)}_2 \rightarrow \tau_2 + \Delta \tau^{(3)}_2.
\]

An immediate consequence from Eq. (16) is that \(\delta t^{(1)}_1 \rightarrow \delta t^{(3)}_1\) and \(\delta t^{(2)}_2 \rightarrow \delta t^{(3)}_2\) as well. Therefore, Eqs. (11) and (12) take the final form:

\[
\Delta_x f_y = \frac{2\delta t^{(3)}_3 - \delta t^{(4)}_1 - (2\delta t^{(2)}_3 - \delta^{(2)}_1)}{(\tau_2 + \Delta \tau^{(2)}_2) \cdot \hat{i}} + \frac{2\delta t^{(3)}_3 - \delta t^{(1)}_2 - (2\delta t^{(3)}_1 - \delta^{(1)}_2)}{(\tau_1 + \Delta \tau^{(3)}_1) \cdot \hat{i}},
\]

and

\[
\Delta_y f_x = \frac{\delta t^{(2)}_1 - \delta t^{(3)}_1}{(\tau_2 + \Delta \tau^{(2)}_2) \cdot \hat{j}} + \frac{\delta t^{(2)}_2 - \delta t^{(3)}_2}{(\tau_1 + \Delta \tau^{(3)}_1) \cdot \hat{j}}.
\]

Equation (10) as derived here supersedes our previous expression for the curl leading to the pseudo-magnetic field [10]. Equation (10) together with Eqs. (17) and (18) were employed in plotting Fig. 4(b) in the main text.

The following approximation helps the reader in better grasping the origin of the curl from differences of changes of on-site potentials upon strain (i.e., a ‘second-order’ differences equation). If we set \(\frac{1}{(\tau_1 + \Delta \tau^{(3)}_1) \cdot \hat{j}} \approx \frac{1}{\tau_1}\) (and a similar approximation for the term involving projection onto \(\hat{j}\)), then the vector projections on the denominator can be carried out easily, and the finite-differences curl takes the following rather intuitive form:

\[
|\Delta \times \mathbf{f}| = \Delta_x f_y - \Delta_y f_x = \frac{4}{\alpha_0}\left[\left(\delta t^{(3)}_3 - \delta t^{(3)}_1\right) + \left(\delta t^{(3)}_2 - \delta t^{(3)}_1\right)\right].
\]

This way:

\[
B_s = -2\sqrt{3}\frac{\phi_0}{\pi a_o^2} \times \left((\delta t^{(3)}_3 - \delta t^{(3)}_1) + (\delta t^{(3)}_2 - \delta t^{(3)}_1)\right)\hat{n},
\]

(\(\hat{n} = \hat{z}\) is the local normal; all constants were defined before [10]; \(a_0 = 1.391\) at 1 Kelvin), and the curl finally becomes Eq. 4 in the main text:

\[
-\mu_B B_s = 2\sqrt{3}g\frac{\hbar}{4me} \frac{\phi_0}{\alpha_o^2} \times \left((\delta t^{(3)}_3 - \delta t^{(3)}_1) + (\delta t^{(3)}_2 - \delta t^{(3)}_1)\right).
\]

\(g\) is the Landé factor, which we set equal to 2. The Landé factor \(g\), along with \(m_e\) – the electron mass – are external parameters of the theory. The prefactor is dimensionless:

\[
2\sqrt{3}g\frac{\hbar}{4me} \frac{\phi_0}{\alpha_o^2} = 2\sqrt{3}\frac{\hbar}{4me} a_o^2 \simeq 2.5.
\]

\(B_s\) changes sign upon sublattice exchange or \(K\)–point exchange. Eq. (15) is related to the staggered DOS observed experimentally, giving additional insight as to how the discrete geometry of graphene couples to its electronic properties.

**Consequences for spin-orbit coupling estimates.** The concepts presented in the main text can be used for an accurate determination of the spin-orbit coupling \(\Delta(r_i)\) induced by curvature. In the absence of strain \(\Delta(r_i) \propto H_D(r_i)\) [41, 50]. An estimate from \(H_D\) in Fig. 2(c) in the main text yields \(-0.2\) meV < \(\Delta < 0.2\) meV [11]. We note that \(\Delta(r_i)\) changes sign with \(H_B\). The proportionality between \(H_D\) and \(\Delta\) depends on hopping invariants that decay exponentially with distance: A more general expression for \(\Delta(r_i)\) must depend on the metric \(g\) as well.

\(H_D\) increases by an order of magnitude and changes sign in between Figs. 2(c) and 3(c) in the main text, making \(|\Delta| \lesssim 2\) meV under central load – even when ignoring effects due to \(g\). As we employed a smearing parameter \(\sigma = 5\) meV in plotting LDOS curves, we were unable to resolve spin-obit coupling, which was hence ignored in the main text.
[41] D. Huertas-Hernando, F. Guinea and A. Brataas, Phys. Rev. B 74, 155426 (2006).
[42] A. A. Pacheco Sanjuan, M. Mehboudi, E. O. Harriss, H. Terrones and S. Barraza-Lopez, ACS Nano, DOI: 10.1021/nn406532z. (2014).
[43] M. Neek-Amal, L. Covaci, K. Shakouri, and F. M. Peeters, Phys. Rev. B 88, 115428 (2013).
[44] A. I. Bobenko, P. Schröder, J. M. Sullivan, and G. M. Ziegler, eds., Discrete Differential Geometry, vol. 38 of Oberwolfach Seminars (Springer, Germany, 2008), 1st ed.
[45] A. I. Bobenko and Y. B. Suris, Discrete Differential Geometry: Integrable Structure. (AMS, USA, 2009), 1st ed.
[46] Z. Xu and G. Xu, Comp. Math. Appl. 57, 1187 (2009).
[47] See supplementary information.
[48] K. K. Gomes, W. Mar, W. Ko, F. Guinea and H. C. Manoharan, Nature 483, 306 (2012).
[49] F. Cirak, M. Ortiz and P. Schröder, Int. J. Numer. Meth. Engng. 47, 2039 (2000).
[50] T. Ando, J. Phys. Soc. Jp. 69, 1757 (2000).
[51] M. I. Katsnelson. Graphene: Carbon in two dimensions. Cambridge U. Press (2012).
[52] S.-M. Choi, S.-H. Jhi and Y.-W. Son, Phys. Rev. B 81, 081407 (2010).
[53] V. Lukose, R. Shankar and G. Baskaran, Phys. Rev. Lett. 98, 116802 (2007).
[54] K.-J. Kim, Ya. M. Blanter and K.-H. Ahn, Phys. Rev. B 84, 081401(R) (2011); G. M. M. Wakker, R. P. Tiwari and M. Blaauwoer, Phys. Rev. B 84, 195427 (2011).