Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information: Single-Layer Structures of a_{100}- and b_{010}-Gallenene: A Tight-Binding Approach

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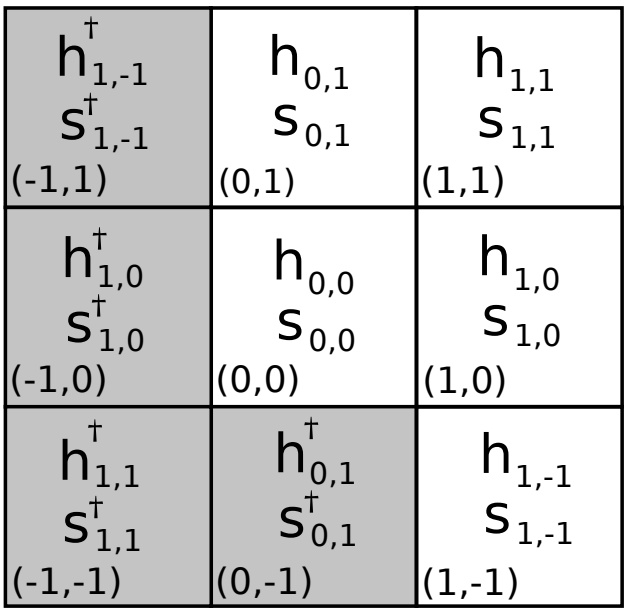

FIG. S.1. Schematic representation of the TB model for a typical 2D material. The white cells indicate independent unit cells.

I. EXPLICIT FORM FOR THE TIGHT-BINDING HAMILTONIAN AND OVERLAP MATRIX

Theoretically the electronic properties of any structure can be described using a simple TB model where the core electrons form fully filled valence bands. We can find a set of orbitals which are only slightly perturbed by the neighbouring atoms and that are responsible for the bands near the Fermi level. Therefore, the mono electric wave function in a typical periodic system can be expressed as a Linear Combination of Atomic Orbitals (LCAO). The main assumption for our TB model is that the dominant contribution comes from nearest unit-cells and that other contributions can be neglected. Fig. S.1 represents the schematic TB model for two dimentional systems.

The system is assumed to be infinite, but using LCAO we are able to limit the system up to a finite number of atoms and a finite number of orbitals per atom which allows us to apply the Bloch theorem. We use these orbitals as the basis set to represent the wave function. The Bloch function with a well-defined $\mathbf{k}$ vector can be generally expanded as linear combinations of the orbitals ϕ as follows

$$\psi_k(\mathbf{r}) = \sum_{\nu'} \sum_{i'} c_{i'\nu'}(k)\phi_{\nu,k}(\mathbf{r} - \mathbf{r}_i), \tag{S1}$$

in which i and ν run over the atoms in the unit cell and the orbitals s, p_x, p_y, and p_z, respectively. In the case of b_{100}-Gallenene and b_{010}-Gallenene we have four orbitals per atom and so 16 orbitals per unit cell. $\phi_{\nu,\mathbf{k}}(\mathbf{r})$ is defined as following

$$\phi_{\nu,\mathbf{k}}(\mathbf{r}) = \sum_{n\in\mathbb{Z}} \sum_{m\in\mathbb{Z}} e^{i\mathbf{k}.\mathbf{R}_{n,m}} \varphi_\nu(\mathbf{r} - \mathbf{R}_{n,m}) \tag{S2}$$

where $\mathbf{R}_{n,m}$ is the discrete translation vector of the unit cell at (m, n). We limit the interactions up to the first nearest unit cell (See Fig. S.1). The mono-electronic Hamiltonian H and the overlap matrix S may be rewritten as

$$\mathbf{H} = \sum_{n=-1}^{1} \sum_{m=-1}^{1} \mathbf{h}_{n,m} e^{i(nak_x + mbk_y)} \tag{S3}$$

and

$$\mathbf{S} = \sum_{n=-1}^{1} \sum_{m=-1}^{1} \mathbf{s}_{n,m} e^{i(nak_x + mbk_y)} \,. \tag{S4}$$

Since $\mathbf{H}$ and $\mathbf{S}$ are Hermitian, we have

$$\begin{aligned}
\mathbf{h}_{-1,0} = \mathbf{h}_{1,0}^\dagger \,, \mathbf{h}_{0,-1} = \mathbf{h}_{0,1}^\dagger \,, \\
\mathbf{h}_{-1,-1} = \mathbf{h}_{1,1}^\dagger \,, \mathbf{h}_{-1,1} = \mathbf{h}_{1,-1}^\dagger \,, \\
\mathbf{s}_{-1,0} = \mathbf{s}_{1,0}^\dagger \,, \mathbf{s}_{0,-1} = \mathbf{s}_{0,1}^\dagger \,, \\
\mathbf{s}_{-1,-1} = \mathbf{s}_{1,1}^\dagger \,, \mathbf{s}_{-1,1} = \mathbf{s}_{1,-1}^\dagger \,.
\end{aligned} \tag{S5}$$

As shown in Fig. S.1 we have only five independent matrices and need to determine the matrices $\mathbf{h}$ and $\mathbf{s}$ for the cells at $(0, 0)$, $(1, 0)$, $(0, 1)$, $(1, 1)$ and $(-1, 1)$. We calculate the Hamiltonian matrix and extract the matrices $\mathbf{h}$ and $\mathbf{s}$ by using the SK coefficients presented in the main paper.

II. TIGHT-BINDING HAMILTONIAN FOR a_{100}-GALLENENE

a_{100}-Gallenene has four atoms per unit cell. Table S.I represents the indices and atomic positions of this structure.

index	x	y	z
1	1.328	4.653	0
2	2.607	2.327	0
3	5.263	2.327	0
4	6.541	0	0

TABLE S.I. The indices and positions of the atoms of a_{100}-Gallenene are in units of $\mathring{A}$ which are used in the construction of the TB model.

In the case of a_{100}-Gallenene we found the SK coefficients in an orthogonal basis set. So the energy bands can be found by finding the eigen values of the hamiltonian mentioned in Eq. (S3). Using the SK integrals presented in the main paper we found the matrices as follows

$$\mathbf{h}_{0,0} = \begin{array}{c} \begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\ \begin{pmatrix} -3.934 & 0 & 0 & 0 & -1.304 & -0.773 & 1.407 & 0 & 0.0159 & 0.029 & -0.017 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.969 & 0 & 0 & 0.773 & 0.092 & -1.220 & 0 & -0.029 & 0.153 & -0.125 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.992 & 0 & -1.407 & -1.220 & 1.642 & 0 & 0.017 & -0.125 & 0.016 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.377 & 0 & 0 & 0 & -0.579 & 0 & 0 & 0 & -0.058 & 0 & 0 & 0 & 0 \\ -1.304 & 0.773 & -1.407 & 0 & -3.934 & 0 & 0 & 0 & -1.304 & -1.605 & 0 & 0 & 0.016 & 0.029 & -0.017 & 0 \\ -0.773 & 0.092 & -1.220 & 0 & 0 & 2.969 & 0 & 0 & 1.605 & 2.313 & 0.001 & 0 & -0.029 & 0.153 & -0.125 & 0 \\ 1.407 & -1.220 & 1.642 & 0 & 0 & 0 & 2.992 & 0 & 0 & 0.001 & -0.579 & 0 & 0.017 & -0.125 & 0.016 & 0 \\ 0 & 0 & 0 & -0.579 & 0 & 0 & 0 & 1.377 & 0 & 0 & 0 & -0.579 & 0 & 0 & 0 & -0.058 \\ 0.016 & -0.029 & 0.017 & 0 & -1.304 & 1.605 & 0 & 0 & -3.934 & 0 & 0 & 0 & -1.304 & -0.773 & 1.407 & 0 \\ 0.029 & 0.153 & -0.125 & 0 & -1.605 & 2.313 & 0.001 & 0 & 0 & 2.969 & 0 & 0 & 0.773 & 0.092 & -1.220 & 0 \\ -0.017 & -0.125 & 0.016 & 0 & 0 & 0.001 & -0.579 & 0 & 0 & 0 & 2.992 & 0 & -1.407 & -1.220 & 1.642 & 0 \\ 0 & 0 & 0 & -0.058 & 0 & 0 & 0 & -0.579 & 0 & 0 & 0 & 1.377 & 0 & 0 & 0 & -0.579 \\ 0 & 0 & 0 & 0 & 0.016 & -0.029 & 0.017 & 0 & -1.304 & 0.773 & -1.407 & 0 & -3.934 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.029 & 0.153 & -0.125 & 0 & -0.773 & 0.092 & -1.220 & 0 & 0 & 2.969 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.017 & -0.125 & 0.016 & 0 & 1.407 & -1.220 & 1.642 & 0 & 0 & 0 & 2.992 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.058 & 0 & 0 & 0 & -0.579 & 0 & 0 & 0 & 1.377 \end{pmatrix} \begin{array}{c} s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{array} \end{array}$$

$$
\mathbf{h}_{1,0} = \begin{array}{cccccccccccccccc|c}
s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
0.016 & 0.029 & 0.017 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
-0.029 & 0.153 & 0.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
-0.017 & 0.125 & 0.016 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
0 & 0 & 0 & -0.058 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
0 & 0 & 0 & 0 & 0.016 & 0.029 & 0.017 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
0 & 0 & 0 & 0 & -0.029 & 0.153 & 0.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
0 & 0 & 0 & 0 & -0.017 & 0.125 & 0.016 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.058 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z
\end{array}
$$

$$
\mathbf{h}_{0,1} = \begin{array}{cccccccccccccccc|c}
s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & \\
\hline
0.016 & 0 & 0.034 & 0 & -1.304 & -0.773 & -1.407 & 0 & 0.016 & 0.029 & 0.017 & 0 & 0 & 0 & 0 & 0 & s \\
0 & -0.058 & 0 & 0 & 0.773 & 0.092 & 1.220 & 0 & -0.029 & 0.153 & 0.125 & 0 & 0 & 0 & 0 & 0 & p_x \\
-0.034 & 0 & 0.227 & 0 & 1.407 & 1.220 & 1.642 & 0 & -0.017 & 0.125 & 0.016 & 0 & 0 & 0 & 0 & 0 & p_y \\
0 & 0 & 0 & -0.058 & 0 & 0 & 0 & -0.579 & 0 & 0 & 0 & -0.058 & 0 & 0 & 0 & 0 & p_z \\
0 & 0 & 0 & 0 & 0.016 & 0 & 0.034 & 0 & 0 & 0 & 0 & 0 & 0.016 & 0.029 & 0.017 & 0 & s \\
0 & 0 & 0 & 0 & 0 & -0.058 & 0 & 0 & 0 & 0 & 0 & 0 & -0.029 & 0.153 & 0.125 & 0 & p_x \\
0 & 0 & 0 & 0 & -0.034 & 0 & 0.227 & 0 & 0 & 0 & 0 & 0 & -0.017 & 0.125 & 0.016 & 0 & p_y \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.058 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.058 & p_z \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.016 & 0 & 0.034 & 0 & -1.304 & -0.773 & -1.407 & 0 & s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.058 & 0 & 0 & 0.773 & 0.092 & 1.220 & 0 & p_x \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.034 & 0 & 0.227 & 0 & 1.407 & 1.220 & 1.642 & 0 & p_y \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.058 & 0 & 0 & 0 & -0.579 & p_z \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.0159 & 0 & 0.034 & 0 & s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.058 & 0 & 0 & p_x \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.034 & 0 & 0.227 & 0 & p_y \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.058 & p_z
\end{array}
$$

$$
\mathbf{h}_{1,-1} = \begin{array}{c}
\begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\
\left(\begin{array}{cccccccccccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.016 & 0.029 & -0.017 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.029 & 0.153 & -0.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.017 & -0.125 & 0.016 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -0.058 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1.304 & -1.605 & 0 & 0 & 0.016 & 0.029 & -0.017 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1.605 & 2.313 & -0.001 & 0 & -0.029 & 0.153 & -0.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -0.001 & -0.579 & 0 & 0.017 & -0.125 & 0.016 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -0.579 & 0 & 0 & 0 & -0.058 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right)
\begin{array}{c} s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{array}
\end{array}
$$

and $\mathbf{h}_{1,1} = \mathbf{s}_{-1,-1} = \mathbf{0}$. All the values are given in units of eV.

III. TIGHT-BINDING HAMILTONIAN AND OVERLAP MATRIX FOR $\mathbf{b}_{010}$-GALLENENE

We presented the SK integrals for the b_{010}-Gallenene in a non-orthogonal basis set. The Hamiltonian that governs the dynamics of the electron is given by Eq. (S3) and the overlap matrix is expressed by Eq. (S4). Assuming again that the contribution dominate up to the secound nearest neighbor. The Schrödinger equation for this system has now been transformed into the form of a generalized eigenvalue equation as follows

$$
\sum_{\nu'}\sum_{i'}[H_{i\nu,i'\nu'} - \epsilon_k S_{i\nu,i'\nu'}]c_{i'\nu'}(k) = 0\,, \tag{S6}
$$

where $c_{i'\nu'}(k)$ is the eigen vector of the system. As presents in Table S.I, b_{010}-Gallenene has four atoms per unit cell.

Using the SK integrals in the main paper we can calculate the Hamiltonian and overlap matrices as following

index	x	y	z
1	0	1.908	0
2	0	4.368	1.193
3	2.372	0.552	0
4	2.372	3.012	1.193

TABLE S.II. The indices and positions of the atoms of b_{010}-Gallenene are in units of $\mathring{A}$.

$$\mathbf{h}_{0,0} = \begin{array}{c} \begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\ \begin{pmatrix} -4.378 & 0 & 0 & 0 & -1.176 & 0 & -2.117 & -1.027 & -1.003 & -1.881 & 1.076 & 0 & -1.176 & -1.941 & -0.903 & -0.976 \\ 0 & -0.099 & 0 & 0 & 0 & -0.795 & 0 & 0 & 1.881 & 1.302 & -1.123 & 0 & 1.941 & 0.63 & 0.663 & 0.717 \\ 0 & 0 & 0.601 & 0 & 2.117 & 0 & 0.901 & 0.823 & -1.076 & -1.123 & -0.02 & 0 & 0.903 & 0.663 & -0.486 & 0.334 \\ 0 & 0 & 0 & 0.682 & 1.027 & 0 & 0.823 & -0.396 & 0 & 0 & 0 & -0.662 & 0.976 & 0.717 & 0.334 & -0.434 \\ -1.176 & 0 & 2.117 & 1.027 & -4.378 & 0 & 0 & 0 & 0.303 & -0.074 & 0.12 & 0.037 & -1.003 & -1.881 & 1.076 & 0 \\ 0 & -0.795 & 0 & 0 & 0 & -0.099 & 0 & 0 & 0.074 & 0.119 & -0.293 & -0.092 & 1.881 & 1.302 & -1.123 & 0 \\ -2.117 & 0 & 0.901 & 0.823 & 0 & 0 & 0.601 & 0 & -0.12 & -0.293 & 0.408 & 0.147 & -1.076 & -1.123 & -0.02 & 0 \\ -1.027 & 0 & 0.823 & -0.396 & 0 & 0 & 0 & 0.682 & -0.037 & -0.092 & 0.147 & -0.017 & 0 & 0 & 0 & -0.662 \\ -1.003 & 1.881 & -1.076 & 0 & 0.303 & 0.074 & -0.12 & -0.037 & -4.378 & 0 & 0 & 0 & -1.176 & 0 & -2.117 & -1.027 \\ -1.881 & 1.302 & -1.123 & 0 & -0.074 & 0.119 & -0.293 & -0.092 & 0 & -0.099 & 0 & 0 & 0 & -0.795 & 0 & 0 \\ 1.076 & -1.123 & -0.02 & 0 & 0.12 & -0.293 & 0.408 & 0.147 & 0 & 0 & 0.601 & 0 & 2.117 & 0 & 0.901 & 0.823 \\ 0 & 0 & 0 & -0.662 & 0.037 & -0.092 & 0.147 & -0.017 & 0 & 0 & 0 & 0.682 & 1.027 & 0 & 0.823 & -0.396 \\ -1.176 & 1.941 & 0.903 & 0.976 & -1.003 & 1.881 & -1.076 & 0 & -1.176 & 0 & 2.117 & 1.027 & -4.378 & 0 & 0 & 0 \\ -1.941 & 0.63 & 0.663 & 0.717 & -1.881 & 1.302 & -1.123 & 0 & 0 & -0.795 & 0 & 0 & 0 & -0.099 & 0 & 0 \\ -0.903 & 0.663 & -0.486 & 0.334 & 1.076 & -1.123 & -0.02 & 0 & -2.117 & 0 & 0.901 & 0.823 & 0 & 0 & 0.601 & 0 \\ -0.976 & 0.717 & 0.334 & -0.434 & 0 & 0 & 0 & -0.662 & -1.027 & 0 & 0.823 & -0.396 & 0 & 0 & 0 & 0.682 \end{pmatrix} \\ \begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \end{array}$$

$$\mathbf{h}_{1,0} = \begin{array}{c} \begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\ \begin{pmatrix} -0.147 & -0.113 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.113 & 0.608 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -0.03 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.03 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.147 & -0.113 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.113 & 0.608 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -0.03 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.03 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1.003 & -1.881 & -1.076 & 0 & 0.303 & -0.074 & -0.12 & -0.037 & -0.147 & -0.113 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1.881 & 1.302 & 1.123 & 0 & 0.074 & 0.119 & 0.293 & 0.092 & 0.113 & 0.608 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1.076 & 1.123 & -0.02 & 0 & 0.12 & 0.293 & 0.408 & 0.147 & 0 & 0 & -0.03 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.662 & 0.037 & 0.092 & 0.147 & -0.017 & 0 & 0 & 0 & -0.03 & 0 & 0 & 0 & 0 \\ -1.176 & -1.941 & 0.903 & 0.976 & -1.003 & -1.881 & -1.076 & 0 & 0 & 0 & 0 & 0 & -0.147 & -0.113 & 0 & 0 \\ 1.941 & 0.63 & -0.663 & -0.717 & 1.881 & 1.302 & 1.123 & 0 & 0 & 0 & 0 & 0 & 0.113 & 0.608 & 0 & 0 \\ -0.903 & -0.663 & -0.486 & 0.334 & 1.076 & 1.123 & -0.02 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.03 & 0 \\ -0.976 & -0.717 & 0.334 & -0.434 & 0 & 0 & 0 & -0.662 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.03 \end{pmatrix} \\ \begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \end{array}$$

$$
\mathbf{h}_{0,1} = \begin{array}{c|cccccccccccccccc|c}
 & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & \\
\hline
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.147 & -0.063 & -0.094 & 0 & 0 & 0 & 0 & 0 & s \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.063 & 0.166 & 0.294 & 0 & 0 & 0 & 0 & 0 & p_x \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.094 & 0.294 & 0.412 & 0 & 0 & 0 & 0 & 0 & p_y \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.03 & 0 & 0 & 0 & 0 & p_z \\
 & -1.176 & 0 & -2.117 & 1.027 & 0 & 0 & 0 & 0 & -1.176 & -1.941 & -0.903 & 0.976 & -0.147 & -0.063 & -0.094 & 0 & s \\
 & 0 & -0.795 & 0 & 0 & 0 & 0 & 0 & 0 & 1.941 & 0.63 & 0.663 & -0.717 & 0.063 & 0.166 & 0.294 & 0 & p_x \\
 & 2.117 & 0 & 0.901 & -0.823 & 0 & 0 & 0 & 0 & 0.903 & 0.663 & -0.486 & -0.334 & 0.094 & 0.294 & 0.412 & 0 & p_y \\
 & -1.027 & 0 & -0.823 & -0.396 & 0 & 0 & 0 & 0 & -0.976 & -0.717 & -0.334 & -0.434 & 0 & 0 & 0 & -0.03 & p_z \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
 & 0.303 & 0.074 & -0.12 & 0.037 & 0 & 0 & 0 & 0 & -1.176 & 0 & -2.117 & 1.027 & 0 & 0 & 0 & 0 & s \\
 & -0.074 & 0.119 & -0.293 & 0.092 & 0 & 0 & 0 & 0 & 0 & -0.795 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
 & 0.12 & -0.293 & 0.408 & -0.147 & 0 & 0 & 0 & 0 & 2.117 & 0 & 0.901 & -0.823 & 0 & 0 & 0 & 0 & p_y \\
 & -0.037 & 0.092 & -0.147 & -0.017 & 0 & 0 & 0 & 0 & -1.027 & 0 & -0.823 & -0.396 & 0 & 0 & 0 & 0 & p_z
\end{array}
$$

$$
\mathbf{h}_{1,1} = \begin{array}{c|cccccccccccccccc|c}
 & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & \\
\hline
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
 & 0.303 & -0.074 & -0.12 & 0.037 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
 & 0.074 & 0.119 & 0.293 & -0.092 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
 & 0.12 & 0.293 & 0.408 & -0.147 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
 & -0.037 & -0.092 & -0.147 & -0.017 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z
\end{array}
$$

$$
\mathbf{h}_{1,-1} = \begin{array}{c}
\begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.147 & -0.063 & 0.094 & 0 & -1.176 & -1.941 & 0.903 & -0.976 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.063 & 0.166 & -0.294 & 0 & 1.941 & 0.63 & -0.663 & 0.717 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.094 & -0.294 & 0.412 & 0 & -0.903 & -0.663 & -0.486 & -0.334 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -0.03 & 0.976 & 0.717 & -0.334 & -0.434 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -0.147 & -0.063 & 0.094 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.063 & 0.166 & -0.294 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -0.094 & -0.294 & 0.412 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.03 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\end{array}
\begin{array}{c} \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{array}
$$

$$
\mathbf{s}_{0,0} = \begin{array}{c}
\begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\
\begin{pmatrix}
1 & 0 & 0 & 0 & 0.017 & 0 & 0.127 & 0.062 & 0.03 & 0.178 & -0.102 & 0 & 0.017 & 0.116 & 0.054 & 0.059 \\
0 & 1 & 0 & 0 & 0 & 0.082 & 0 & 0 & -0.178 & -0.185 & 0.26 & 0 & -0.116 & -0.224 & -0.142 & -0.154 \\
0 & 0 & 1 & 0 & -0.127 & 0 & -0.281 & -0.176 & 0.102 & 0.26 & 0.121 & 0 & -0.054 & -0.142 & 0.016 & -0.072 \\
0 & 0 & 0 & 1 & -0.062 & 0 & -0.176 & -0.004 & 0 & 0 & 0 & 0.27 & -0.059 & -0.154 & -0.072 & 0.005 \\
0.017 & 0 & -0.127 & -0.062 & 1 & 0 & 0 & 0 & -0.034 & -0.002 & 0.002 & 0.001 & 0.03 & 0.178 & -0.102 & 0 \\
0 & 0.082 & 0 & 0 & 0 & 1 & 0 & 0 & 0.002 & -0.028 & 0.004 & 0.001 & -0.178 & -0.185 & 0.26 & 0 \\
0.127 & 0 & -0.281 & -0.176 & 0 & 0 & 1 & 0 & -0.002 & 0.004 & -0.032 & -0.002 & 0.102 & 0.26 & 0.121 & 0 \\
0.062 & 0 & -0.176 & -0.004 & 0 & 0 & 0 & 1 & -0.001 & 0.001 & -0.002 & -0.026 & 0 & 0 & 0 & 0.27 \\
0.03 & -0.178 & 0.102 & 0 & -0.034 & 0.002 & -0.002 & -0.001 & 1 & 0 & 0 & 0 & 0.017 & 0 & 0.127 & 0.062 \\
0.178 & -0.185 & 0.26 & 0 & -0.002 & -0.028 & 0.004 & 0.001 & 0 & 1 & 0 & 0 & 0 & 0.082 & 0 & 0 \\
-0.102 & 0.26 & 0.121 & 0 & 0.002 & 0.004 & -0.032 & -0.002 & 0 & 0 & 1 & 0 & -0.127 & 0 & -0.281 & -0.176 \\
0 & 0 & 0 & 0.27 & 0.001 & 0.001 & -0.002 & -0.026 & 0 & 0 & 0 & 1 & -0.062 & 0 & -0.176 & -0.004 \\
0.017 & -0.116 & -0.054 & -0.059 & 0.03 & -0.178 & 0.102 & 0 & 0.017 & 0 & -0.127 & -0.062 & 1 & 0 & 0 & 0 \\
0.116 & -0.224 & -0.142 & -0.154 & 0.178 & -0.185 & 0.26 & 0 & 0 & 0.082 & 0 & 0 & 0 & 1 & 0 & 0 \\
0.054 & -0.142 & 0.016 & -0.072 & -0.102 & 0.26 & 0.121 & 0 & 0.127 & 0 & -0.281 & -0.176 & 0 & 0 & 1 & 0 \\
0.059 & -0.154 & -0.072 & 0.005 & 0 & 0 & 0 & 0.27 & 0.062 & 0 & -0.176 & -0.004 & 0 & 0 & 0 & 1
\end{pmatrix}
\end{array}
\begin{array}{c} \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{array}
$$

$$
\mathbf{s}_{1,0} = \begin{array}{c}
\begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\
\begin{pmatrix}
0.027 & 0.015 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.015 & -0.071 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.055 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.055 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.027 & 0.015 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -0.015 & -0.071 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.055 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.055 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.03 & 0.178 & 0.102 & 0 & -0.034 & -0.002 & -0.002 & -0.001 & 0.027 & 0.015 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.178 & -0.185 & -0.26 & 0 & 0.002 & -0.028 & -0.004 & -0.001 & -0.015 & -0.071 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.102 & -0.26 & 0.121 & 0 & 0.002 & -0.004 & -0.032 & -0.002 & 0 & 0 & 0.055 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.27 & 0.001 & -0.001 & -0.002 & -0.026 & 0 & 0 & 0 & 0.055 & 0 & 0 & 0 & 0 \\
0.017 & 0.116 & -0.054 & -0.059 & 0.03 & 0.178 & 0.102 & 0 & 0 & 0 & 0 & 0 & 0.027 & 0.015 & 0 & 0 \\
-0.116 & -0.224 & 0.142 & 0.154 & -0.178 & -0.185 & -0.26 & 0 & 0 & 0 & 0 & 0 & -0.015 & -0.071 & 0 & 0 \\
0.054 & 0.142 & 0.016 & -0.072 & -0.102 & -0.26 & 0.121 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.055 & 0 \\
0.059 & 0.154 & -0.072 & 0.005 & 0 & 0 & 0 & 0.27 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.055
\end{pmatrix}
\end{array}
\begin{array}{c} \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{array}
$$

$$
\mathbf{s}_{0,1} = \begin{array}{c}
\begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.027 & 0.008 & 0.012 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.008 & 0.016 & -0.058 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.012 & -0.058 & -0.032 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.055 & 0 & 0 & 0 & 0 \\
0.017 & 0 & 0.127 & -0.062 & 0 & 0 & 0 & 0 & 0.017 & 0.116 & 0.054 & -0.059 & 0.027 & 0.008 & 0.012 & 0 \\
0 & 0.082 & 0 & 0 & 0 & 0 & 0 & 0 & -0.116 & -0.224 & -0.142 & 0.154 & -0.008 & 0.016 & -0.058 & 0 \\
-0.127 & 0 & -0.281 & 0.176 & 0 & 0 & 0 & 0 & -0.054 & -0.142 & 0.016 & 0.072 & -0.012 & -0.058 & -0.032 & 0 \\
0.062 & 0 & 0.176 & -0.004 & 0 & 0 & 0 & 0 & 0.059 & 0.154 & 0.072 & 0.005 & 0 & 0 & 0 & 0.055 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.034 & 0.002 & -0.002 & 0.001 & 0 & 0 & 0 & 0 & 0.017 & 0 & 0.127 & -0.062 & 0 & 0 & 0 & 0 \\
-0.002 & -0.028 & 0.004 & -0.001 & 0 & 0 & 0 & 0 & 0 & 0.082 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.002 & 0.004 & -0.032 & 0.002 & 0 & 0 & 0 & 0 & -0.127 & 0 & -0.281 & 0.176 & 0 & 0 & 0 & 0 \\
-0.001 & -0.001 & 0.002 & -0.026 & 0 & 0 & 0 & 0 & 0.062 & 0 & 0.176 & -0.004 & 0 & 0 & 0 & 0
\end{pmatrix}
\end{array}
\begin{array}{c} \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{array}
$$

$$
\mathbf{s}_{1,1} = \begin{array}{c}
\begin{matrix} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{matrix} \\
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.034 & -0.002 & -0.002 & 0.001 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.002 & -0.028 & -0.004 & 0.001 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.002 & -0.004 & -0.032 & 0.002 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.001 & 0.001 & 0.002 & -0.026 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\end{array}
\begin{matrix} \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{matrix}
$$

$$
\mathbf{s}_{1,-1} = \begin{array}{c}
\begin{matrix} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{matrix} \\
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.027 & 0.008 & -0.012 & 0 & 0.017 & 0.116 & -0.054 & 0.059 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.008 & 0.016 & 0.058 & 0 & -0.116 & -0.224 & 0.142 & -0.154 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.012 & 0.058 & -0.032 & 0 & 0.054 & 0.142 & 0.016 & 0.072 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.055 & -0.059 & -0.154 & 0.072 & 0.005 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.027 & 0.008 & -0.012 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -0.008 & 0.016 & 0.058 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.012 & 0.058 & -0.032 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.055 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\end{array}
\begin{matrix} \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{matrix}
$$

In the case of orthogonal TB model for b_{010}-Gallenene the energy bands can be found by finding the eigen values of the hamiltonian mentioned in Eq. (S3). Using the SK integrals presented in the main paper we found the matrices as follows

$$
\mathbf{h}_{0,0} = \begin{array}{c}
\begin{array}{cccccccccccccccc}
s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z
\end{array} \\
\begin{pmatrix}
-3.188 & 0 & 0 & 0 & -0.771 & 0 & -1.289 & -0.625 & -0.612 & -1.61 & 0.921 & 0 & -0.771 & -1.182 & -0.55 & -0.595 \\
0 & 1.052 & 0 & 0 & 0 & -0.831 & 0 & 0 & 1.61 & 0.572 & -0.689 & 0 & 1.182 & 0.516 & 0.627 & 0.677 \\
0 & 0 & 1.907 & 0 & 1.289 & 0 & 0.771 & 0.777 & -0.921 & -0.689 & -0.24 & 0 & 0.55 & 0.627 & -0.539 & 0.315 \\
0 & 0 & 0 & 1.393 & 0.625 & 0 & 0.777 & -0.454 & 0 & 0 & 0 & -0.634 & 0.595 & 0.677 & 0.315 & -0.49 \\
-0.771 & 0 & 1.289 & 0.625 & -3.188 & 0 & 0 & 0 & 0.013 & 0.037 & -0.06 & -0.019 & -0.612 & -1.61 & 0.921 & 0 \\
0 & -0.831 & 0 & 0 & 0 & 1.052 & 0 & 0 & -0.037 & -0.019 & 0.233 & 0.073 & 1.61 & 0.572 & -0.689 & 0 \\
-1.289 & 0 & 0.771 & 0.777 & 0 & 0 & 1.907 & 0 & 0.06 & 0.233 & -0.249 & -0.117 & -0.921 & -0.689 & -0.24 & 0 \\
-0.625 & 0 & 0.777 & -0.454 & 0 & 0 & 0 & 1.393 & 0.019 & 0.073 & -0.117 & 0.089 & 0 & 0 & 0 & -0.634 \\
-0.612 & 1.61 & -0.921 & 0 & 0.013 & -0.037 & 0.06 & 0.019 & -3.188 & 0 & 0 & 0 & -0.771 & 0 & -1.289 & -0.625 \\
-1.61 & 0.572 & -0.689 & 0 & 0.037 & -0.019 & 0.233 & 0.073 & 0 & 1.052 & 0 & 0 & 0 & -0.831 & 0 & 0 \\
0.921 & -0.689 & -0.24 & 0 & -0.06 & 0.233 & -0.249 & -0.117 & 0 & 0 & 1.907 & 0 & 1.289 & 0 & 0.771 & 0.777 \\
0 & 0 & 0 & -0.634 & -0.019 & 0.073 & -0.117 & 0.089 & 0 & 0 & 0 & 1.393 & 0.625 & 0 & 0.777 & -0.454 \\
-0.771 & 1.182 & 0.55 & 0.595 & -0.612 & 1.61 & -0.921 & 0 & -0.771 & 0 & 1.289 & 0.625 & -3.188 & 0 & 0 & 0 \\
-1.182 & 0.516 & 0.627 & 0.677 & -1.61 & 0.572 & -0.689 & 0 & 0 & -0.831 & 0 & 0 & 0 & 1.052 & 0 & 0 \\
-0.55 & 0.627 & -0.539 & 0.315 & 0.921 & -0.689 & -0.24 & 0 & -1.289 & 0 & 0.771 & 0.777 & 0 & 0 & 1.907 & 0 \\
-0.595 & 0.677 & 0.315 & -0.49 & 0 & 0 & 0 & -0.634 & -0.625 & 0 & 0.777 & -0.454 & 0 & 0 & 0 & 1.393
\end{pmatrix}
\end{array}
\begin{array}{c}
s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z
\end{array}
$$

$$
\mathbf{h}_{1,0} = \begin{array}{c}
\begin{array}{cccccccccccccccc}
s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z
\end{array} \\
\begin{pmatrix}
-0.176 & 0.042 & 0 & 0 & -0.249 & -0.152 & -0.079 & -0.038 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.042 & -0.163 & 0 & 0 & 0.152 & 0.122 & 0.053 & 0.026 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.126 & 0 & 0.079 & 0.053 & 0.047 & 0.013 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.126 & 0.038 & 0.026 & 0.013 & 0.026 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.249 & -0.152 & 0.079 & 0.038 & -0.176 & 0.042 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.152 & 0.122 & -0.053 & -0.026 & -0.042 & -0.163 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.079 & -0.053 & 0.047 & 0.013 & 0 & 0 & 0.126 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.038 & -0.026 & 0.013 & 0.026 & 0 & 0 & 0 & 0.126 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.612 & -1.61 & -0.921 & 0 & 0.013 & 0.037 & 0.06 & 0.019 & -0.176 & 0.042 & 0 & 0 & -0.249 & -0.152 & -0.079 & -0.038 \\
1.61 & 0.572 & 0.689 & 0 & -0.037 & -0.019 & -0.233 & -0.073 & -0.042 & -0.163 & 0 & 0 & 0.152 & 0.122 & 0.053 & 0.026 \\
0.921 & 0.689 & -0.24 & 0 & -0.06 & -0.233 & -0.249 & -0.117 & 0 & 0 & 0.126 & 0 & 0.079 & 0.053 & 0.047 & 0.013 \\
0 & 0 & 0 & -0.634 & -0.019 & -0.073 & -0.117 & 0.089 & 0 & 0 & 0 & 0.126 & 0.038 & 0.026 & 0.013 & 0.026 \\
-0.771 & -1.182 & 0.55 & 0.595 & -0.612 & -1.61 & -0.921 & 0 & -0.249 & -0.152 & 0.079 & 0.038 & -0.176 & 0.042 & 0 & 0 \\
1.182 & 0.516 & -0.627 & -0.677 & 1.61 & 0.572 & 0.689 & 0 & 0.152 & 0.122 & -0.053 & -0.026 & -0.042 & -0.163 & 0 & 0 \\
-0.55 & -0.627 & -0.539 & 0.315 & 0.921 & 0.689 & -0.24 & 0 & -0.079 & -0.053 & 0.047 & 0.013 & 0 & 0 & 0.126 & 0 \\
-0.595 & -0.677 & 0.315 & -0.49 & 0 & 0 & 0 & -0.634 & -0.038 & -0.026 & 0.013 & 0.026 & 0 & 0 & 0 & 0.126
\end{pmatrix}
\end{array}
\begin{array}{c}
s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z
\end{array}
$$

$$\mathbf{h}_{0,1} = \begin{array}{c} \begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\ \begin{pmatrix} -0.025 & 0 & 0.098 & 0 & 0 & 0 & 0 & 0 & -0.176 & 0.023 & 0.035 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.108 & 0 & 0 & 0 & 0 & 0 & 0 & -0.023 & 0.037 & -0.133 & 0 & 0 & 0 & 0 & 0 \\ -0.098 & 0 & -0.1 & 0 & 0 & 0 & 0 & 0 & -0.035 & -0.133 & -0.074 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.108 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.126 & 0 & 0 & 0 & 0 \\ -0.771 & 0 & -1.289 & 0.625 & -0.025 & 0 & 0.098 & 0 & -0.771 & -1.182 & -0.55 & 0.595 & -0.176 & 0.023 & 0.035 & 0 \\ 0 & -0.831 & 0 & 0 & 0 & 0.108 & 0 & 0 & 1.182 & 0.516 & 0.627 & -0.677 & -0.023 & 0.037 & -0.133 & 0 \\ 1.289 & 0 & 0.771 & -0.777 & -0.098 & 0 & -0.1 & 0 & 0.55 & 0.627 & -0.539 & -0.315 & -0.035 & -0.133 & -0.074 & 0 \\ -0.625 & 0 & -0.777 & -0.454 & 0 & 0 & 0 & 0.108 & -0.595 & -0.677 & -0.315 & -0.49 & 0 & 0 & 0 & 0.126 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.025 & 0 & 0.098 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.108 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.098 & 0 & -0.1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.108 & 0 & 0 & 0 & 0 \\ 0.013 & -0.037 & 0.06 & -0.019 & 0 & 0 & 0 & 0 & -0.771 & 0 & -1.289 & 0.625 & -0.025 & 0 & 0.098 & 0 \\ 0.037 & -0.019 & 0.233 & -0.073 & 0 & 0 & 0 & 0 & 0 & -0.831 & 0 & 0 & 0 & 0.108 & 0 & 0 \\ -0.06 & 0.233 & -0.249 & 0.117 & 0 & 0 & 0 & 0 & 1.289 & 0 & 0.771 & -0.777 & -0.098 & 0 & -0.1 & 0 \\ 0.019 & -0.073 & 0.117 & 0.089 & 0 & 0 & 0 & 0 & -0.625 & 0 & -0.777 & -0.454 & 0 & 0 & 0 & 0.108 \end{pmatrix} \\ \begin{array}{c} s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{array} \end{array}$$

$$\mathbf{h}_{1,-1} = \begin{array}{c} \begin{array}{cccccccccccccccc} s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 & -0.249 & -0.152 & 0.079 & -0.038 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.152 & 0.122 & -0.053 & 0.026 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.079 & -0.053 & 0.047 & -0.013 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.038 & 0.026 & -0.013 & 0.026 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -0.176 & 0.023 & -0.035 & 0 & -0.771 & -1.182 & 0.55 & -0.595 & 0 & 0 & 0 & 0 & -0.249 & -0.152 & 0.079 & -0.038 \\ -0.023 & 0.037 & 0.133 & 0 & 1.182 & 0.516 & -0.627 & 0.677 & 0 & 0 & 0 & 0 & 0.152 & 0.122 & -0.053 & 0.026 \\ 0.035 & 0.133 & -0.074 & 0 & -0.55 & -0.627 & -0.539 & -0.315 & 0 & 0 & 0 & 0 & -0.079 & -0.053 & 0.047 & -0.013 \\ 0 & 0 & 0 & 0.126 & 0.595 & 0.677 & -0.315 & -0.49 & 0 & 0 & 0 & 0 & 0.038 & 0.026 & -0.013 & 0.026 \\ 0 & 0 & 0 & 0 & -0.176 & 0.023 & -0.035 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.023 & 0.037 & 0.133 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.035 & 0.133 & -0.074 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.126 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \\ \begin{array}{c} s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \\ s \\ p_x \\ p_y \\ p_z \end{array} \end{array}$$

$$\mathbf{h}_{1,1} = \begin{array}{cccccccccccccccc|c}
s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & s & p_x & p_y & p_z & \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_x \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_y \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & p_z \\
0.013 & 0.037 & 0.06 & -0.019 & 0 & 0 & 0 & 0 & -0.249 & -0.152 & -0.079 & 0.038 & 0 & 0 & 0 & 0 & s \\
-0.037 & -0.019 & -0.233 & 0.073 & 0 & 0 & 0 & 0 & 0.152 & 0.122 & 0.053 & -0.026 & 0 & 0 & 0 & 0 & p_x \\
-0.06 & -0.233 & -0.249 & 0.117 & 0 & 0 & 0 & 0 & 0.079 & 0.053 & 0.047 & -0.013 & 0 & 0 & 0 & 0 & p_y \\
0.019 & 0.073 & 0.117 & 0.089 & 0 & 0 & 0 & 0 & -0.038 & -0.026 & -0.013 & 0.026 & 0 & 0 & 0 & 0 & p_z
\end{array}$$

Note that the indices of the elements of the Hamiltonian and the overlap matrix are the same as the indices presented in Table S.II. Other elements of the coupling matrices can be found from the relations Eq. (S5).

IV. BAND STRUCTURE OF THE GALLENENE NANO RIBBONS WITH DIFFERENT WIDTHS

In this section we show the benefit of the TB model. When we have a TB model we can generate the Hamiltonian for different structures. Using the hamiltonian matrices for two dimentional a_{100}-Gallenene and b_{010}-Gallenene presented in section I one can generate the hamiltonian for unit-cell of a ribbon of any size and their coupling matrices between first unit-cell and neighbor unit-cells. The structure of the nanoribbons for both armchair and zigzag directions were presented in the main paper in Fig. 5. The width of the nanoribbon can be determined by the parameter N. We calculated the band structure of different nanoribbons to show the behavior of the energy bands as a function of N. In the following we show the results for $N = 2, 3, 4, 5, 6$ and 7.

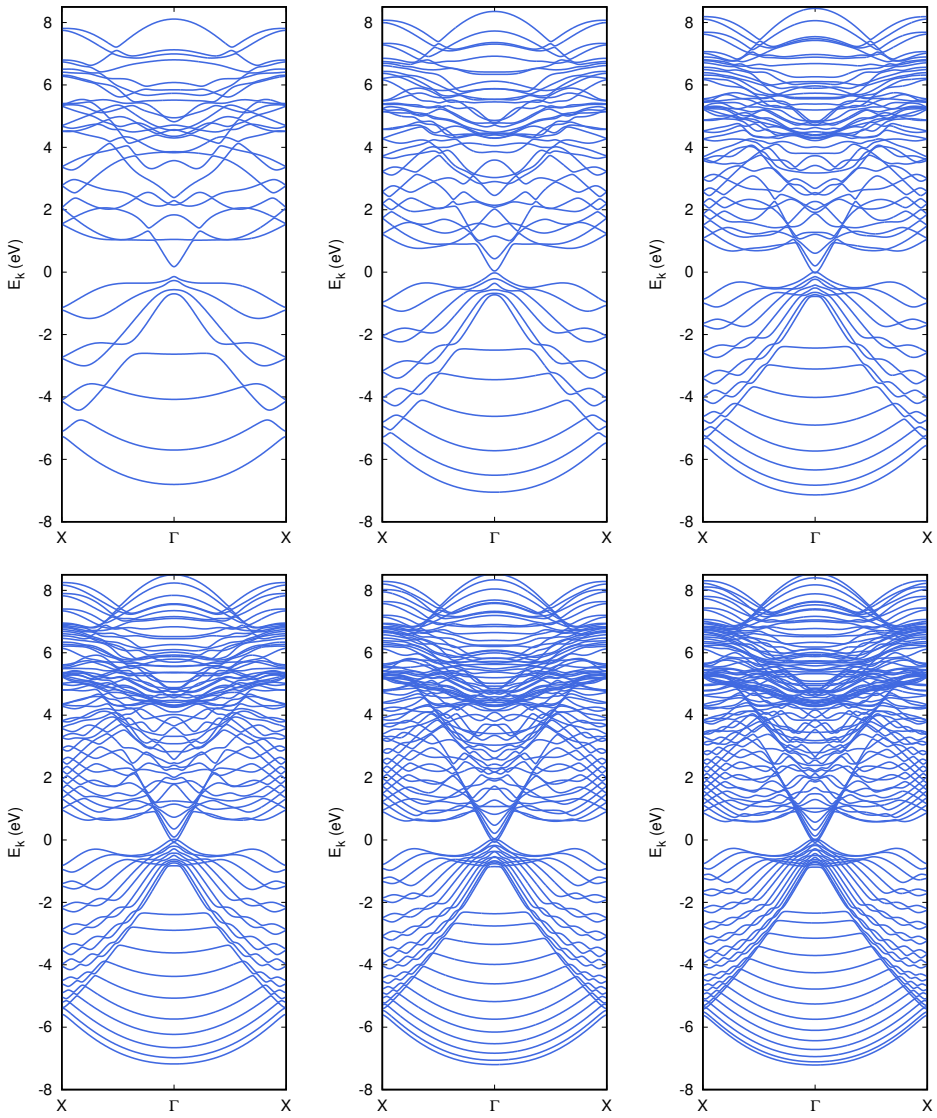

FIG. S.2. Bands Structure of b_{010}-Gallenene AC nanoribbon for N = 2, 3, 4, 5, 6 and 7, respectively.

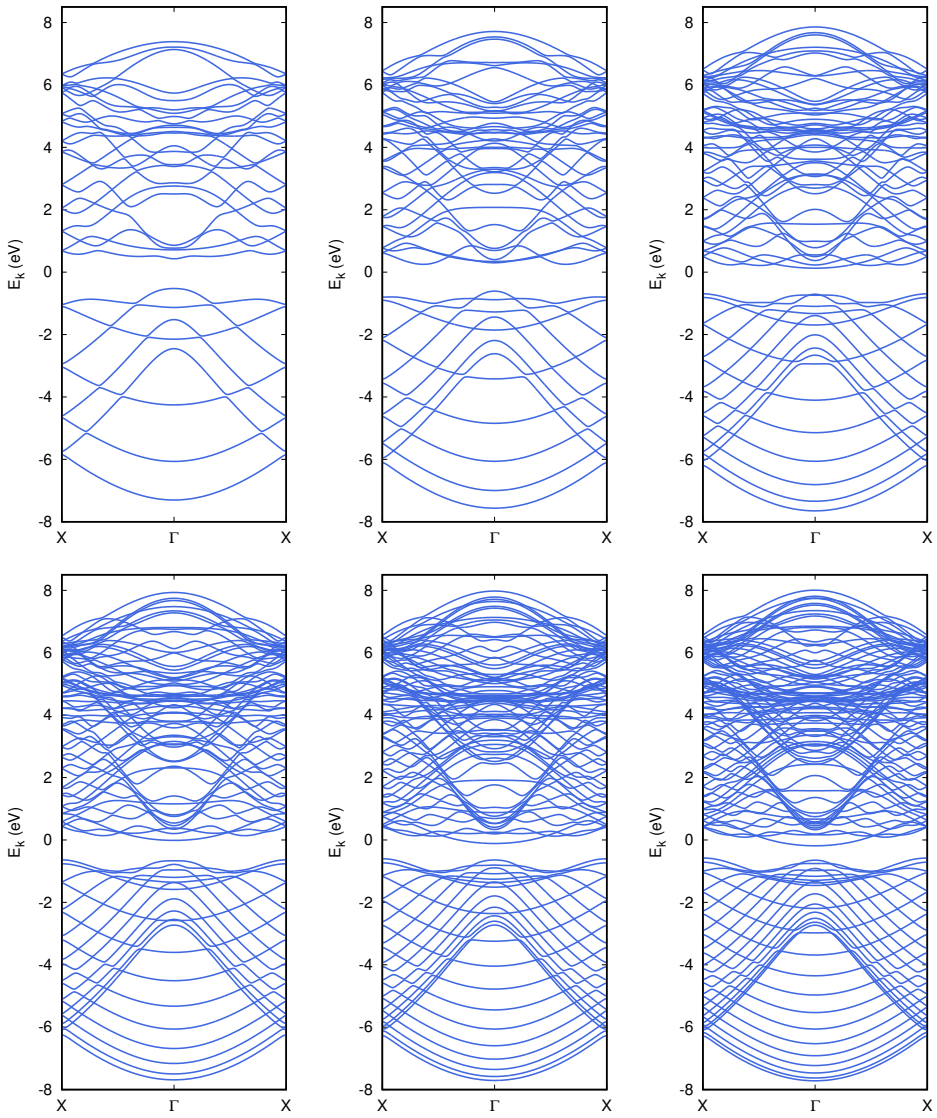

FIG. S.3. Bands Structure of b_{010}-Gallenene ZZ nanoribbon for N = 2, 3, 4, 5, 6 and 7, respectively.

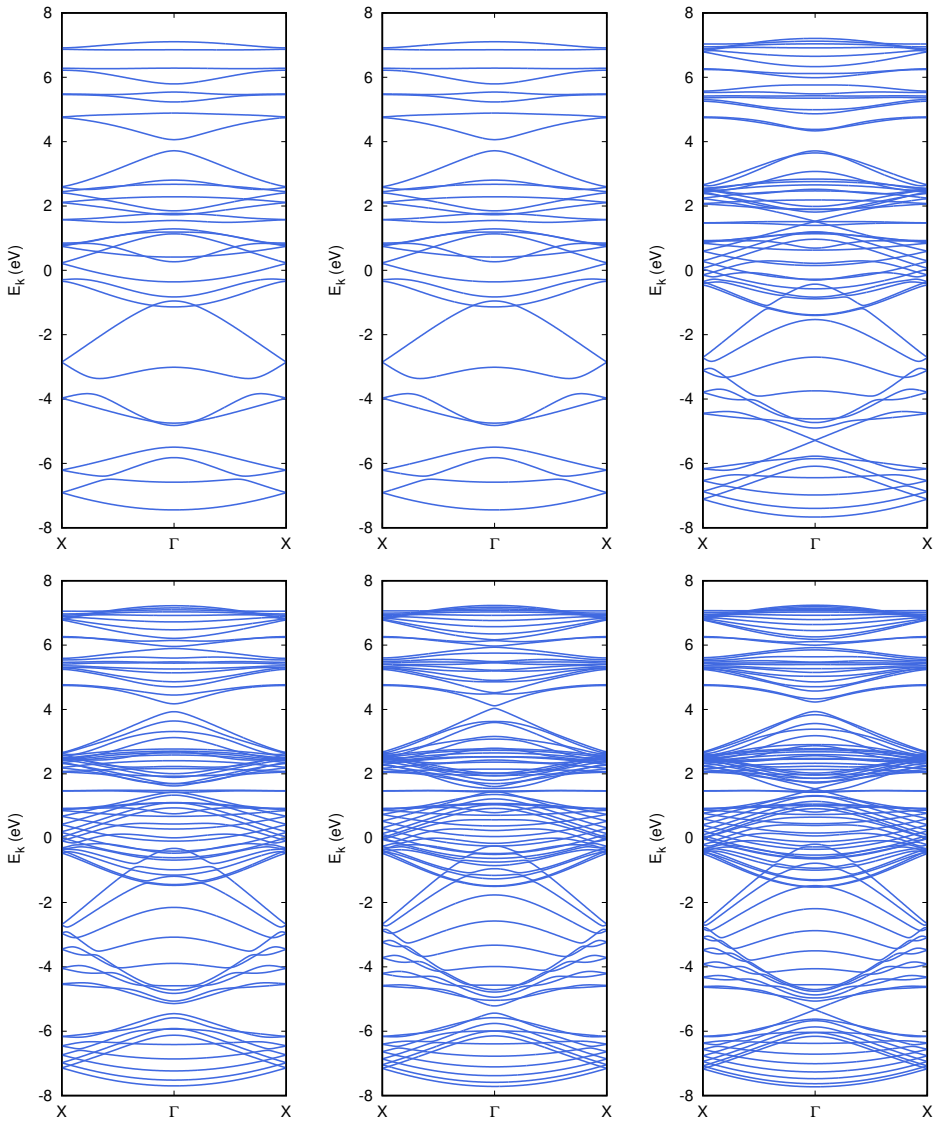

FIG. S.4. Bands Structure of a_{100}-Gallenene AC nanoribbon for N = 2, 3, 4, 5, 6 and 7, respectively.

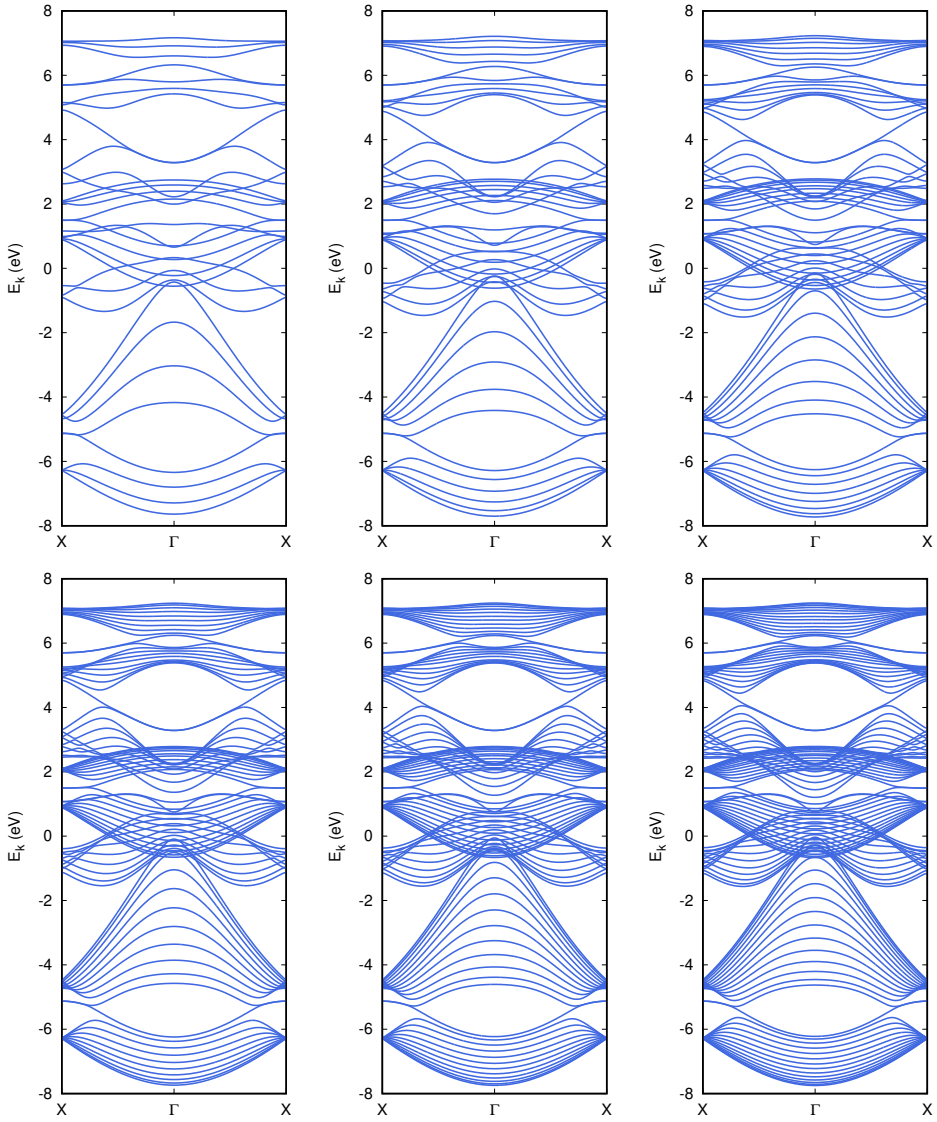

FIG. S.5. Bands Structure of a_{100}-Gallenene ZZ nanoribbon for N = 2, 3, 4, 5, 6 and 7, respectively.