RESEARCH ARTICLE

Flat band localization due to self-localized orbital

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Supporting Information

I The Calculation of electron waveguides with finite difference method

In the main text, the Hamiltonian of the electron waveguide is

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + U(r), \tag{S1}$$

where $U(r)$ is the periodic confinement potential of the waveguide. As shown in Fig. S1, we divide the coordinate domain into a uniform grid. The blue solid lines are the potential boundary, outside which $U_{ij} \equiv U(r_{ij}) = \infty$. Here, $r_{ij} = (x_i, y_j)$ is the coordinate of the grid sites. $U_{ij} = 0$ inside the electron waveguide (gray region). The red solid lines are the two connecting edges between adjacent unit cells. The wave function at r_{ij} is denoted as $\psi_{ij} = \psi(x_i, y_j)$.
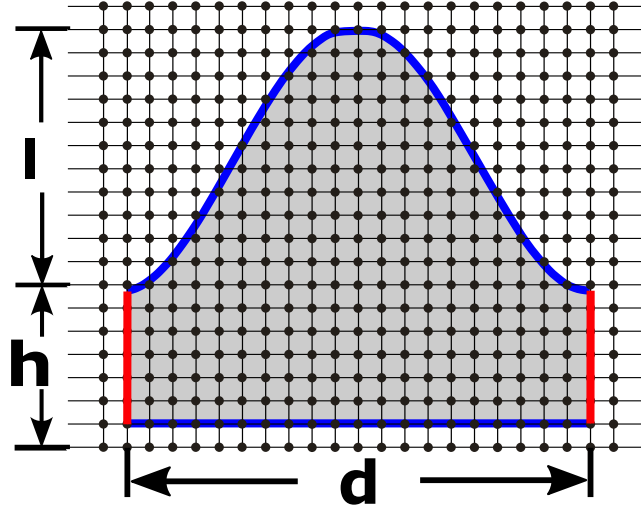

FIG. S1. Calculation of an electron waveguide with the method of finite differences. $U(r_{ij})$ is zero inside the electron waveguide (the gray region), and the blue lines are the boundary of the waveguide. The red lines are the connecting edges between unit cells of the waveguide, i.e. the periodic boundaries.

Using the finite difference method, we have

$$\frac{\partial^2}{\partial x^2}\psi(x,y) = \frac{1}{a^2}(\psi_{i-1,j} - 2\psi_{ij} + \psi_{i+1,j}),$$

$$\frac{\partial^2}{\partial y^2}\psi(x,y) = \frac{1}{a^2}(\psi_{i,j-1} - 2\psi_{i,j} + \psi_{i,j+1}), \tag{S2}$$

where a is the lattice constant of the grid. The Schrödinger equation becomes

$$E\psi_{i,j} = (4t + U_{i,j})\psi_{i,j} - t\psi_{i+1,j} - t\psi_{i-1,j} - t\psi_{i,j-1} - t\psi_{i,j+1}. \tag{S3}$$

Here, $t = \frac{\hbar^2}{2m} \cdot \frac{1}{a^2}$. We can define a column vector

$$\Phi = (\cdots\cdots\psi_{i,j-1} \;,\; \psi_{i,j} \;,\; \psi_{i,j+1} \cdots\cdots\psi_{i+1,j-1} \;,\; \psi_{i+1,j} \;,\; \psi_{i+1,j+1} \cdots\cdots)^T, \tag{S4}$$

so that the Eq. (S3) can be viewed as a matrix equation. Since that the U_{ij} is infinite outside the potential boundary, the corresponding wave function should be zero. Thus, we only need to consider the wave function on the sites inside the electron waveguide.

Note that U_{ij} for the electron waveguide here is periodic,

$$U(\mathbf{r} + d\mathbf{e}_x) = U(\mathbf{r}). \tag{S4}$$

Here, d is the width of the unit cell of electron waveguide [see also in Fig. 1 (b) of the main text] and $\mathbf{e}_x$ is the unit vector along the x direction. The corresponding eigenfunction is a Bloch wave

$$\psi_k(r_{ij}) = e^{ikx_i}\chi_k(r_{ij}), \tag{S4}$$

where $\chi_k(r_{ij})$ is the periodic function to be determined. Now, the Eq. (S3) is transformed into

$$E\chi_k(r_{ij}) = (4t + U_{ij})\chi_k(r_{ij}) - te^{ika}\chi(r_{i+1,j}) - te^{-ika}\chi_k(r_{i-1,j}) - t\chi_k(r_{i,j+1}) - t\chi_k(r_{i,j-1}). \tag{S5}$$

Finally, we can get the bands and wavefunctions by diagonalizing the Hamiltonian matrix

$$H(k) = \begin{pmatrix} \vdots & & & & \\ U+4t & 0 & -te^{ika} & 0 & 0 \\ & & \vdots & & \\ 0 & U+4t & -t & 0 & 0 \\ & & \vdots & & \\ \cdots -te^{-ika} \cdots & -t & \cdots U+4t \cdots & -te^{ika} \cdots & -t & \cdots \\ & & \vdots & & \\ 0 & 0 & -te^{-ika} & U+4t & 0 \\ & & \vdots & & \\ 0 & 0 & -t & 0 & U+4t \\ & & \vdots & & \end{pmatrix}. \tag{S6}$$

We emphasize that, though a discretized lattice is used for the calculation, the designed waveguide here is essentially a spatially continuous system, and can not be simply equated with a lattice model. It is because that the solutions of a partial difference equation are essentially irrelevant to the discretized lattice, which is just an approximation to assist the calculation. In fact, to solve the Eq. (S1), the discretized lattice is neither necessary nor unique. For example, if we use the finite element method, the choice of discretized lattice is arbitrary. And we even do not need any discretized lattice if the plane wave method is used. In a word, our results here do not rely on any lattice structure, and thus is out of the framework of the flat band lattice model.

In Fig. S2, we also give the geometry parameters of the two electron waveguides in Fig. 1 (e) and (g) of the main text.

II Fermi level and carrier density in the electron waveguide

The Fermi level of the electron waveguide is determined by the charge density of the 2DEG. In experiment, the Fermi level can be controlled by tuning the charge density. Here, we take the electron waveguide given in Fig. 1

FIG. S2.   (a) Parameters of electronic waveguide in Fig. 1 (e) of the main text: $a = 82nm$ and $b = 40nm$. (b) Parameters of electronic waveguide in Fig. 1 (f) of the main text: $c = d = 40nm$ and $r = 10nm$.

(c) for example, where the energy bands are plotted in Fig. 1 (d) of the main text. With the energy bands, we can calculate the DOS and charge density (Fig. S3). If we want the Fermi level in the upper flat band (the sixth bands), the electron density of the 2DEG should be in the region $1.05 \backsim 1.25 \times 10^{11} cm^{-2}$.
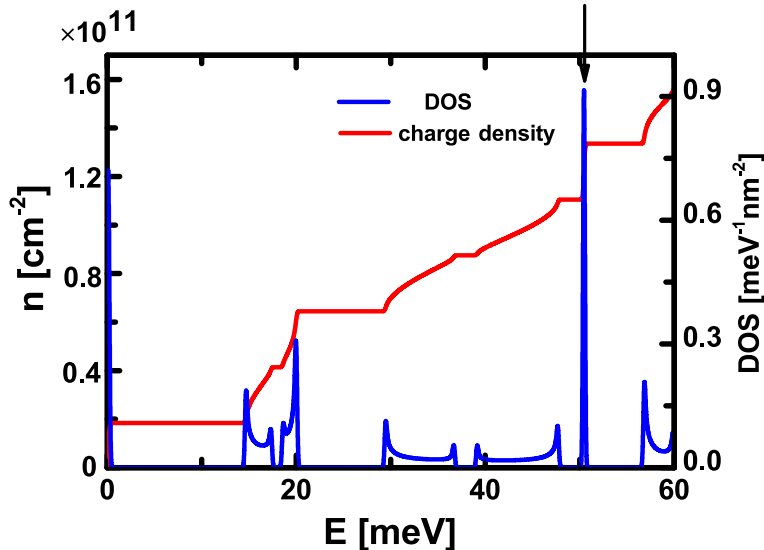

FIG. S3. The charge density and DOS for electric waveguide in Fig. 1 (c) of the main text. The red line is the charge density, and the blue lines are the DOS. The black arrow indicate the position of the flat band of the electron waveguide [the sixth band in Fig. 1 (d) of the main text].

III Band inversion and hybridization induced partially flat band

In Fig. 1 (h) of the main text, we see a small bump appears near the $k = 0$ point in the flat band (red line). Meanwhile, the lower dispersive band get a small flat top in the same region, see the inset of the Fig. 1 (h). So, the flat band here is partially flat here. Actually, the bump as well as the flat top results from a band inversion and hybridization between the flat band the the lower dispersive band, as demonstrated in Fig. S4. In Fig. S4 (a), we replot the Fig. 1 (h) of the main text for convenience. Fig. S4 (b) is the zoomed plot of the band structure, in which a band inversion and hybridization between the flat band (red line) and the 2nd band (blue line) is shown clearly. The 2nd band is below the flat band in the whole Brillouin zone except the bump region (small region nearby k=0). Meanwhile, there is a tiny hybridization between these two bands, which gives rise to a small gap when the two bands cross each other. Thus, we finally get a bump in the flat band and a flat top in the lower dispersive band, see Fig. S4 (b).

To further illustrate such band inversion picture, we plot the wave functions of the two bands at several k points, as marked in Fig. S4 (b). As shown in Fig. S4 (b), the k point 1 is in the flat top of the 2nd band, and its wave function is given in Fig. S4 (c). As a comparison, the wave function of k point 4 at the flat band is plotted in Fig. S4 (e). We see that the wave functions of the k point 1 and 4 are very similar, which are just the self-localized orbitals. It means that the flat top of the 2nd bands is from the self-localized orbital induced flat band. We further plot the wave function of the k point 2 in the bump of the flat band, see Fig. S4 (d), which is clearly different from the self-localized orbital . Actually, it is similar as that in the 2nd band, e.g. the wave function of k point 3 given in Fig. S4 (f).

IV Orbitals of the artificial atom in electron waveguide

In Fig. 2 (b) and (c) of the main text, we plot two orbitals of an isolated artificial atom. The confinement potential $U(r)$ of the isolated atom is given in Fig. 2 (a) of the main text. Here, we plot the lowest six orbitals of this artificial atom together in Fig. S5. The Fig. S5 (a) to (f) correspond to the first to sixth orbitals, respectively. Note that the first orbital [Fig. S5(a)] and the sixth orbital [Fig. S5 (f)] correspond to the lower and upper flat bands in Fig. 1 (d) of the main text, respectively.
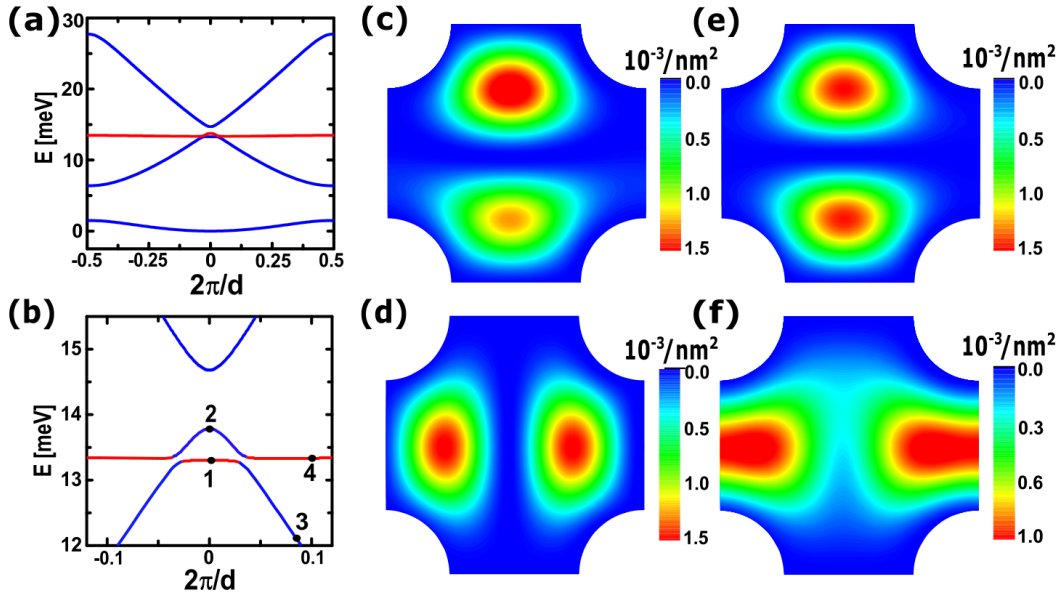
FIG. S4. (a) The same as the Fig.1 (h) of the main text for convenience. (b) The zoomed plot of the band structure, where a band inversion and hybridization between the flat band (red line) and the 2nd band (blue line) is shown clearly. (c) (d) (e) and (f) are wave functions at the k points of 1, 2, 4 and 3, as marked in (b), respectively.
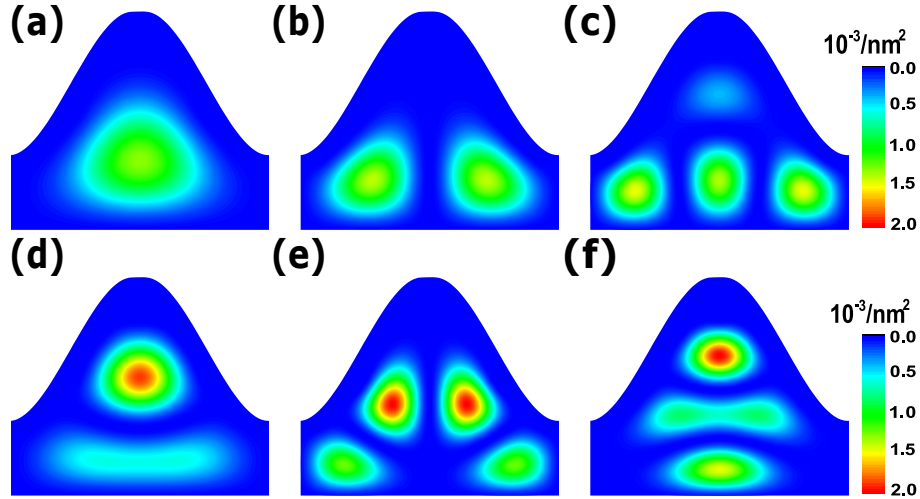

FIG. S5. Orbitals of isolated artificial atom with the confinement potential $U(r)$ which have been shown in Fig.2(a). The lowest six orbitals of this artificial atom are given in (a)-(f).

V   comparison between the bands of the electronic waveguide and that of the metallic waveguide array

In the main text, the electron waveguide in Fig. 1 (c) and the metallic waveguide array [Fig. 3 (c) of the main text] have similar geometry. They thus actually have very similar band structure. Though we calculate the bands of the two systems with different numerical methods, the calculated bands have the same shape. The comparison between the bands of the two system is given in Fig. S6. The bands of the electron waveguides with various geometry parameters are given in Fig. S6 (a), (b) and (c). The corresponding bands of the metallic waveguide arrays are shown in Fig. S6 (d), (e), (f), in which the TE modes are plotted with red solid lines (blue dashed lines are the TM modes). We see that, via carefully choosing the the geometry parameters, the bands of the electron waveguide and the TE modes of the metallic waveguide array can have the same shape [see Fig. S6 (a)/(d); (b)/(e); (c)/(f)]. The geometry is illustrated in Fig. 1 (b) and Fig. 3 (b). The parameters are: (a) $d/h/l = 52/40/26$ nm; (b) $d/h/l = 52/52/26$ nm;
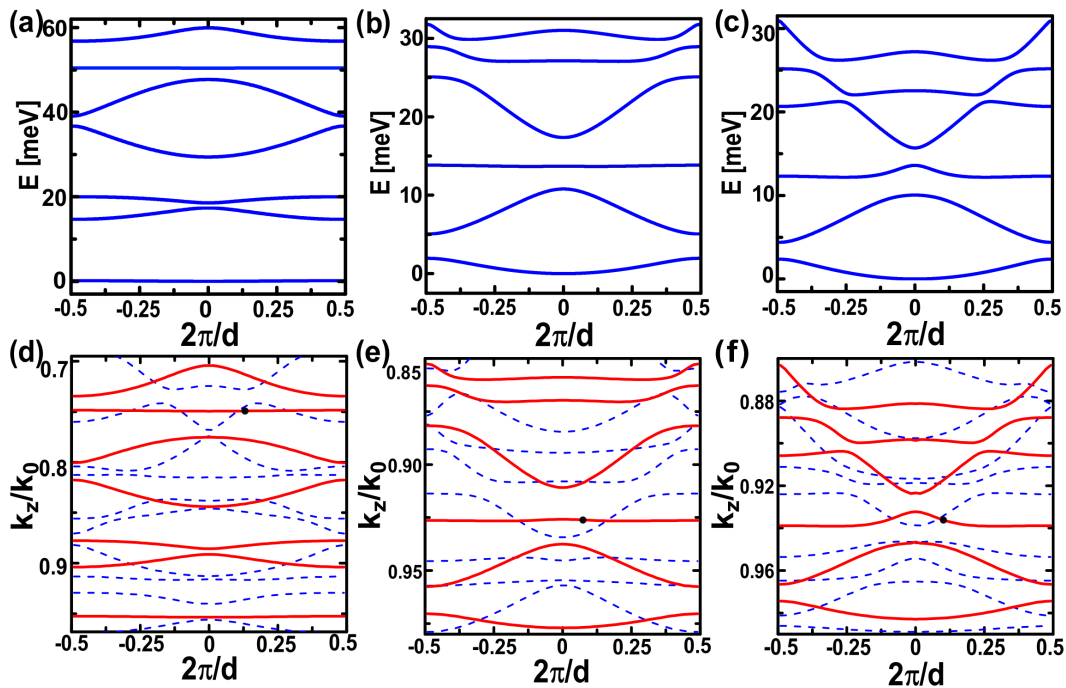
FIG. S6. (a), (b), (c) are the bands of the electron waveguides, the geometry of which is shown in Fig. 1 (b) of the main text; (d), (e), (f) are the bands of the metallic waveguide arrays, the geometry of which is illustrated in Fig. 3 (b) of the main text. Red solid lines are the TE modes, and blue dashed lines are the TM modes. The parameters are: (a) $d/h/l = 52/40/26$ nm; (b) $d/h/l = 52/52/26$ nm; (c) $d/l/h = 52/62/26$ nm; (d) $d/l/h = 16/8/5$ cm; (e) $d/l/h = 16/8/9.2$ cm; (f) $d/l/h = 16/8cm/11.2$ cm.
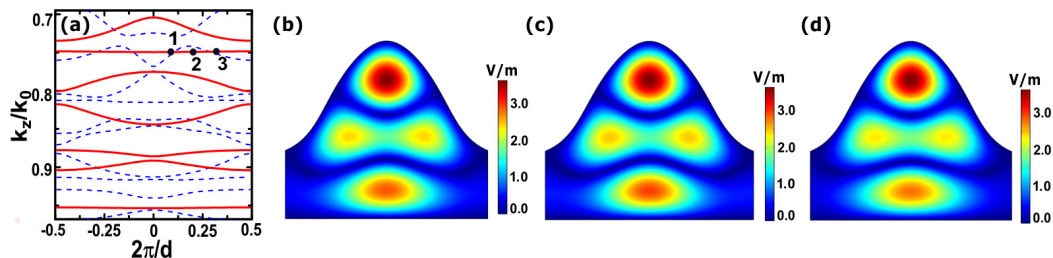
FIG. S7. The eigen-fields of the flat band at different k points. (a) The band diagram. (b), (c) and (d) are the eigen-fields of the k points 1, 2 and 3, as marked in (a).

(c) $d/l/h = 52/62/26$ nm; (d) $d/l/h = 16/8/5$ cm; (e) $d/l/h = 16/8/9.2$ cm; (f) $d/l/h = 16/8cm/11.2$ cm.

VI   Eigen-fields of the flat band in the metallic waveguide array

In the main text, we say that the wave functions of each flat band at various k points are the same, i.e. just the self-localized orbital. Here, we illustrate this point again in the metallic waveguide array. We use the case in Fig. 3 (d) as example, and the eigen-fields at different k point of the flat band are plotted in Fig. S7. Here, Fig. S7 (b), (c), (d) are the eigen-fields of the k point 1, 2, 3 as marked in Fig. S7 (a), respectively. Compared with Fig. 3 (c) of the main text, it is clear that they are just the self-localized orbitals.
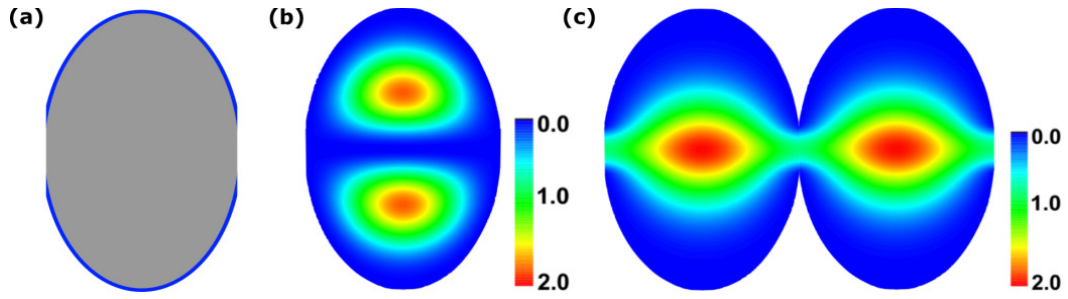
FIG. S8. (a) is the shape of the artificial atom (b) is the artificial orbital of the flat band,(c) is the artificial orbit of the first dispersion band.

VII   Isolated artificial atom of the artificial atom

We plot the typical orbitals of the isolated artificial atom of Fig.1(e) in Fig. S8. Fig. S8 (a) show the shape of the artificial atom in detail. Fig. S8(b) is the artificial orbital of the flat band. The electrons in this orbital actually are strictly localized in each unit cell. In contrast, we also plot the artificial orbit of the first dispersion band in Fig. S8(c). We can see that this wave function is extended.