This Supplementary Information is divided into two sections. In the Sec. I, we firstly report the one-dimensional (1D) numerical results, including the Bloch spectra of the linearized version of the underlying physical model—Gross-Pitaevskii equation with a 1D optical lattice by varying its depth (lattice strength), the physical explanation of the origin of 1D matter-wave dark gap structures confined in the first and second finite band gaps such as dark gap solitons and soliton clusters and their relationships with the corresponding nonlinear Bloch waves; typical examples of the stable and unstable dark gap localized modes are displayed, shown are also for their eigenvalue problems via linear-stability analysis and for their dynamical evolution over time by means of direct simulations.

For the Sec. II of two-dimensional (2D) numerical results, we propose a way to realize the possible 2D optical lattice imprinted with different numbers of bright defects, show contour plots and stable evolutions of the 2D matter-wave fundamental dark gap structures in the form of local defect modes, including the dark gap solitons (in both the 1st and 2nd band gaps) and soliton clusters, and also the stable and unstable evolutions of their vortical counterparts; the dependence $N(\mu)$ is also shown for these vortical dark gap modes.
FIG. 1. (a) Band-gap structure for 1D Bloch waves as a function of $V_0$ (amplitude of optical lattice). (b) The relevant Bloch spectrum at $V_0 = 3$. SIG: semi-infinite gap; 1st BG and 2nd BG: first and second Band gap.

FIG. 2. 1D coherent matter-wave structures within the first band gap with $\mu = 1.8$: (a) nonlinear Bloch wave, (b) dark soliton, and (c) dark soliton cluster; wave structures within the second band gap with $\mu = 3.6$: (d) nonlinear Bloch wave, (e) dark soliton, and (f) dark soliton cluster. The spacing ($\Delta$) between adjacent solitons is $\Delta = 2\pi$ for panels (c,f).

I. SUPPLEMENTARY INFORMATION FOR 1D NUMERICAL RESULTS

Depicted in Fig. 1(a) is the Band-gap structure of 1D optical lattice, as given in the main text, whose form is defined as $V_{OL} = V_0 \sin^2(x)$, with $V_0$ being lattice strength (constant parameter). Besides the intrinsic semi-infinite gap, there are first finite band gap, the second band gap and more by varying the lattice strength $V_0$. For the value of $V_0 = 3$ that we are interested in, its corresponding Bloch spectrum is depicted in Fig. 1(b), from which one can see that it possesses the first two finite band gaps: first band gap and the second one. For simplicity, and without losing generality, we take $V_0 = 3$ for all the 1D cases under study.

Fig. 2 displays the 1D coherent matter-wave structures in forms of nonlinear Bloch waves, dark solitons and dark soliton clusters in the first (top row) and second (bottom row) band gaps respectively. From the comparison between the dark gap localized modes (dark solitons and soliton clusters) and their corresponding nonlinear Bloch waves, we clearly see that the nonlinear Bloch waves are the backgrounds on which all the dark gap modes are located, these modes may hence be called Bloch wave modulated dark gap modes.

Fig. 3 illustrates the time evolution of 1D dark gap solitons via direct numerical simulations of the perturbed solutions (with small initial perturbation adding to the so-found stationary solutions). Fig. 3(a) shows the case of unstable dark gap soliton whose chemical potential $\mu = 1.23$ is close to the band edge, which is consistent with our linear stability analysis in the central panel; it is seen from the bottom panel that the unstable dark gap soliton loses its coherence after evolution of some time, it decays and is repelled to both ends and leaves behind the relevant nonlinear Bloch wave background. Figs. 3(b,c) show respectively the stable ones in first band gap at $\mu = 1.8$ and in the second band gap at $\mu = 3.6$. 

FIG. 3. Profiles, eigenvalues and evolutions (with small initial perturbation) of 1D dark gap solitons: (a) unstable soliton at $\mu = 1.23$; stable solitons at $\mu = 1.8$ (b) and at $\mu = 3.6$ (c). (a,b) for the modes in first band gap, and (c) for the one in the second band gap. The evolutions in the bottom panels start with adding small initial perturbation to the 1D dark gap solitons (the perturbed solutions).

FIG. 4. Profiles (top), eigenvalues (middle) and evolutions (bottom) of 1D dark gap soliton clusters: (a) unstable soliton cluster at $\mu = 1.2$; stable soliton clusters at $\mu = 1.8$ (b, d) and at $\mu = 3.6$ (c). The spacing ($\Delta$) between adjacent solitons is $\Delta = 2\pi$ for (a,b,c) and $\Delta = 3\pi$ for (d). (a,b,d) for the modes in first band gap, and (c) for the one in the second band gap. The evolutions in the bottom panels start with adding small initial perturbation to the 1D dark gap soliton clusters (the perturbed solutions).
We report the evolution of 1D dark gap soliton clusters in Fig. 4. Similar to that of the single dark gap solitons in Fig. 3(a), the same evolution process goes on for the unstable dark gap soliton cluster [see Fig. 4(a)]. Figs. 4(b) and 4(d) show the stable dark gap soliton clusters within the frist band gap, and Fig. 4(c) is for the stable one in the second gap. In particular, we demonstrate that these soliton clusters can be stable modes at different soliton spacing ($\Delta$), e.g., $\Delta = 2\pi$ for Figs. 4(b, c) and $\Delta = 3\pi$ for Fig. 4(d); simulations conclude that stable modes can only present if $\Delta = n\Delta_{\text{latt}} = n\pi$ (with $n \geq 2$), recall that the period of the optical lattice is $\Delta_{\text{latt}} = \pi$.

II. SUPPLEMENTARY INFORMATION FOR 2D NUMERICAL RESULTS

![Fig. 5](image1.png)

FIG. 5. The proposed scheme to generate the defective optical potential—optical lattice with induced single (a) or multiple (b) bright defects, by combing the homogeneous optical lattices (left column) and defects (middle column). Note that the defects should be introduced at the minimum positions of the optical lattices. Perpendicular dashed lines in the top right panel represent two coordinates (x and y), with the intersection corresponds to coordinate origin (0,0).

![Fig. 6](image2.png)

FIG. 6. Contour plots of 2D coherent matter-wave structures: dark gap solitons in first band gap at $\mu = 3.1$ (a) and in second band gap at $\mu = 4.36$ (b), dark gap soliton cluster at $\mu = 3.1$. Panels in the bottom show the evolutions of these coherent dark structures against small initial perturbation (perturbed solutions). Perpendicular dashed lines in panel (a) represent two coordinates (x and y), with the intersection as coordinate origin (0,0).
In this section, we try to explore the existence of 2D matter-wave dark gap structures, including dark gap solitons and soliton clusters as those for their 1D counterparts mentioned above. While we fail after extensive searches, since the considered model with homogeneous optical lattice cannot support any 2D dark gap modes any more. One can borrow the idea that is widely used in the field of optics, where the photonics crystals with different kinds defects can allow for light propagation within the optical band gaps of the underlying linear spectrum, such method is called defect engineering [see the references 40-44 in the main text].

As regards the atomic Bose-Einstein condensate trapped by optical lattices, such method applies too and several types of matter-wave bright gap structures supported by dark defects have been created in a work by Zeng and Malomed [see the reference 49 in the main text], where the bright gap solitons and vortices existed as localized defect modes. Regarding this, one may think that whether the dark gap wave structures can be supported by bright defects. Our numerical calculations verified this conjecture, as will be shown in the following. Considering the fact that, the optical lattices are created by sets of counter-propagating laser beams of which the angle between the polarizations, the relative phase and intensity can be easily tuned, so that one may realize different lattice structures at will, offering great flexibility for ultracold experiments. And in this way, the optical lattices with bright defects can be fabricated as well.

![FIG. 7. Norm $N$ versus chemical potential $\mu$ for 2D matter-wave vortical modes of dark gap soliton clusters composed of thirty-six solitons supported by a perfect optical lattice (a) and by the imperfect optical lattice (b).](image)

![FIG. 8. Evolutions of perturbed solutions in the form of dark gap vortex solitons (vortices): (a) stable mode with vortex charge $m = 1$ at $\mu = 4.36$; (b) unstable mode with $m = 2$ at $\mu = 2.7$. Perpendicular dashed lines in panel (a) denote two coordinates (x and y), with the crossing represents the coordinate origin (0,0).](image)

Having established the way to create such imperfect optical lattices with bright defects, the creation of 2D dark gap solitons and soliton clusters (soliton composites consisted by identical dark gap solitons) and their vortical counterparts is therefore can be envisaged. As described in the main text of the paper, the 2D matter-wave dark gap structures form as localized defect states, with central dips pinning at the bright defects, supported by the balanced effect of the repulsive interatomic interactions, diffraction and the induced optical lattices.
FIG. 9. Evolutions of perturbed solutions representing the vortical modes of dark gap soliton clusters: (a) stable mode with vortex charge \( m = 2 \) at \( \mu = 2.4 \); (b) unstable mode with \( m = 3 \) at \( \mu = 3.4 \). Panels in the central column show the comparison of the initial profiles and the ones after propagating some time.

Evolutions of 2D dark gap solitons relied on the first and second finite band gaps are respectively depicted in Figs. 6(a) and 6(b); and the one for dark gap soliton clusters is depicted Fig. 6(c). These 2D matter-wave dark gap structures are stable nonlinear excitations, corroborated by linear stability analysis and direct numerical simulations, since they are fundamental modes of the considered physical system.

Simulation further proved that, in addition to the fundamental modes mentioned above, the physical system under study also supports a vast variety of 2D matter-wave dark gap solitons carrying topological charge \( m \), including the dark gap vortex solitons and vortical ones of soliton clusters. The relation between norm \( N \) versus chemical potential \( \mu \) for these dark gap vortex structures is summed in Figs. 7(a) and 7(b), separately.

We report the evolutions of dark gap vortex solitons in Figs. 8(a) and 8(b) respectively, for the ones with topological charge \( m = 1 \) and with \( m = 2 \). Numerous simulations verified that such dark gap vortex solitons are stable localized defect modes provided that \( m = 1 \), while unstable at \( m \geq 2 \).

Finally, we report the evolutions of stable and unstable vortical modes of the dark gap soliton clusters carrying topological charge \( m = 2 \) and \( m = 3 \) respectively in Figs. 9(a) and 9(b). For the unstable vortical mode, the dark gap soliton cluster loses its coherence after some time evolution, exchanging energy (amplitude) and phase between each identical solitons; by contrast, everything (in particular, the amplitude and shape) is keeping the same during the evolution, showing good robustness and flexibility of such vortical mode. Our numerical investigations proved that this kind of vortical modes are stable if \( m \leq 2 \), while unstable at \( m \geq 3 \). Other physical descriptions of them could be referred to the main text.