

Supplementary Materials for  
**Acoustofluidic black holes for multifunctional in-droplet  
particle manipulation**

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Tables S1 and S2  
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References

**Other Supplementary Material for this manuscript includes the following:**

Movies S1 to S3

## section S1. Details of numerical models

The governing equation for computing wave fields in the solid domain (56) is

$$-\rho\omega^2\mathbf{u} = \nabla \cdot \mathbf{S} + \mathbf{F}_V e^{i\varphi} \quad (\text{S1})$$

where  $\rho$  is the substrate density,  $\omega$  is the angular frequency,  $\mathbf{u}$  is the displacement vector,  $\mathbf{S}$  is the stress tensor,  $\mathbf{F}_V$  is the volume force vector, and  $\varphi$  is the phase. The quadratic serendipity shape functions are used to simulate displacement fields in the Solid Mechanics interface.

The governing equation for computing acoustic pressure fields in the fluid domain (57, 58) is

$$\nabla^2 p + \left(\frac{\omega}{c_0}\right)^2 p = 0 \quad (\text{S2})$$

where  $p$  is the acoustic pressure and  $c_0$  is the wave speed in water. The quadratic Lagrangian shape functions are used to simulate acoustic pressure fields in the Pressure Acoustics interface. Aside from the coupled droplet-substrate interface, other boundaries of the fluid domain are set to acoustic soft boundaries (59).

After computing the acoustic pressure field, the acoustic velocity  $\mathbf{v}$  in the fluid domain can be computed (57, 58) based on the equation

$$\mathbf{v} = -\frac{\nabla p}{i\omega\rho_0} \quad (\text{S3})$$

where  $\rho_0$  is the water density. With the simulated acoustic pressure and velocity, the acoustic radiation force  $\mathbf{F}_{rad}$  applied on a single particle in the acoustic field can be computed (60) using the equation

$$\mathbf{F}_{rad} = -\nabla \left\{ \frac{4}{3} \pi R_p^3 \left[ \left( -\frac{3\rho_p - 3\rho_o}{2\rho_p + \rho_o} \right) \cdot \frac{1}{2} \rho_o \langle \mathbf{v} \rangle^2 + \left( 1 - \frac{\rho_o c_o^2}{\rho_p c_p^2} \right) \cdot \frac{1}{2} \frac{\langle p \rangle^2}{\rho_o c_o^2} \right] \right\} \quad (\text{S4})$$

where  $R_p$  is the particle radius,  $\rho_p$  is the particle density, and  $c_p$  is the particle material's sound speed.

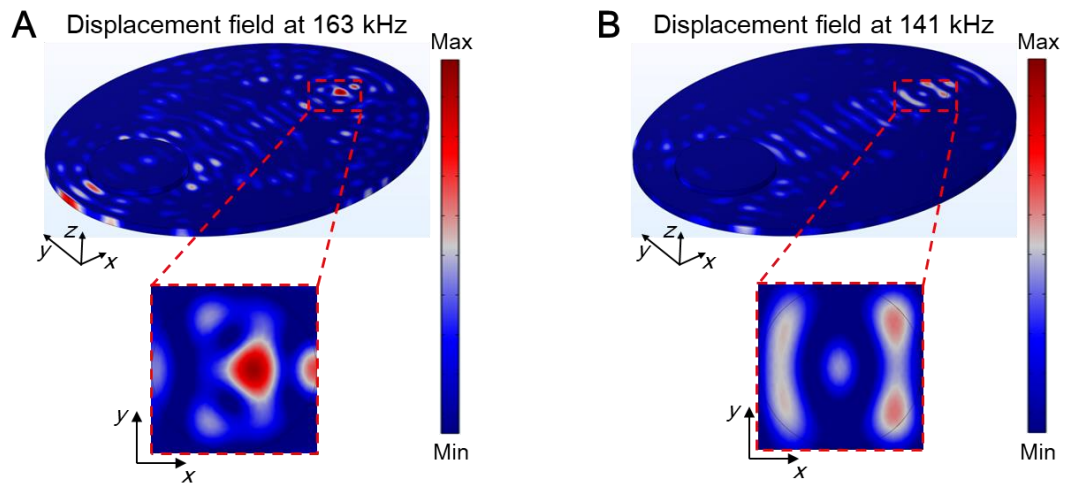
The governing equations for computing acoustic streaming fields in the fluid domain are

$$\nabla \cdot \mathbf{v}_1 = 0 \quad (\text{S5})$$

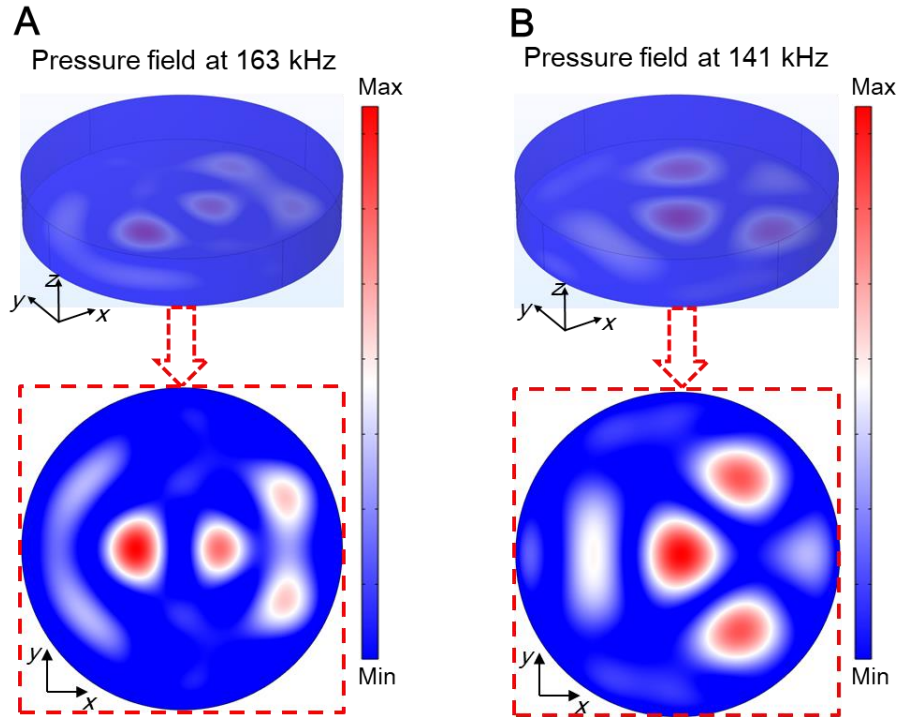
$$\rho_0 (\mathbf{v}_1 \cdot \nabla) \mathbf{v}_1 = \nabla \cdot \left\{ -p_1 \mathbf{I} + \mu \left[ \nabla \mathbf{v}_1 + (\nabla \mathbf{v}_1)^T \right] \right\} + \mathbf{F}_R \quad (\text{S6})$$

$$\mathbf{F}_R = -\rho_0 \langle (\mathbf{v} \cdot \nabla) \mathbf{v} + \mathbf{v} (\nabla \cdot \mathbf{v}) \rangle \quad (\text{S7})$$

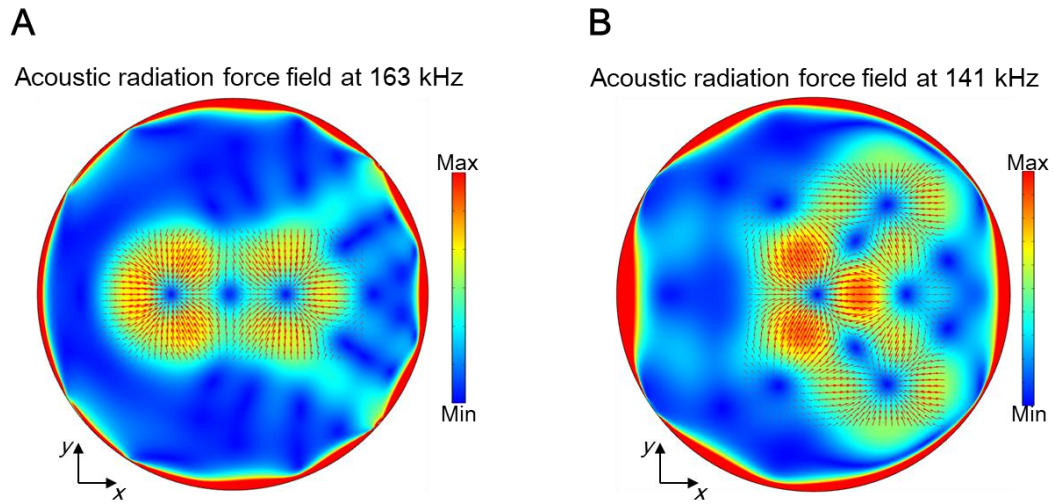
where  $\mathbf{v}_1$  is the acoustic streaming velocity,  $p_1$  is the pressure in the fluid,  $\mu$  is the dynamic viscosity of water, and  $\mathbf{F}_R$  is the body force induced by the acoustic field ( $\langle \rangle$  denotes the time average over a full oscillation time period) (61, 62). The fluid flow discretization is set to P1+P1 (piecewise linear interpolation for velocity and pressure) in the Laminar Flow interface. The coupled droplet-substrate interface is set to a slip boundary (63-65), and other boundaries of the fluid domain are set to no-slip boundaries.



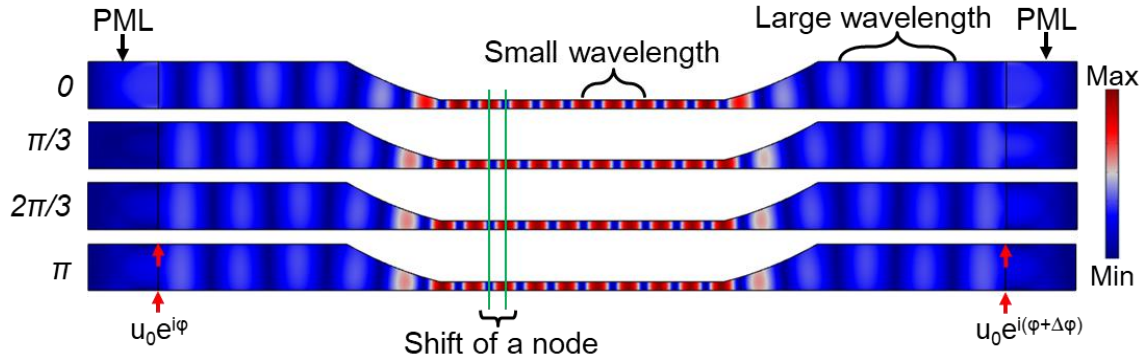
**fig. S1. Simulated out-of-plane displacement amplitude fields for flexural waves generated in an elliptical substrate without an AFBH. (A) Simulation result at 163 kHz. (B) Simulation result at 141 kHz. These simulation results indicate the elliptical boundary can focus wideband flexural waves generated by a circular piezoelectric transducer to a region near the right focal point of the ellipse.**



**fig. S2. Simulated acoustic pressure fields in the fluid domain at different frequencies.** (A) Simulation result at 163 kHz. (B) Simulation result at 141 kHz. Top row: 3D views of the simulated pressure fields. Bottom row: 2D views of the simulated pressure fields at the fluid-solid interface. These simulation results indicate that our AFBH can change in-droplet pressure fields and pressure antinode numbers by altering excitation frequencies. These features allow our AFBH-based device to achieve different in-droplet particle distributions.

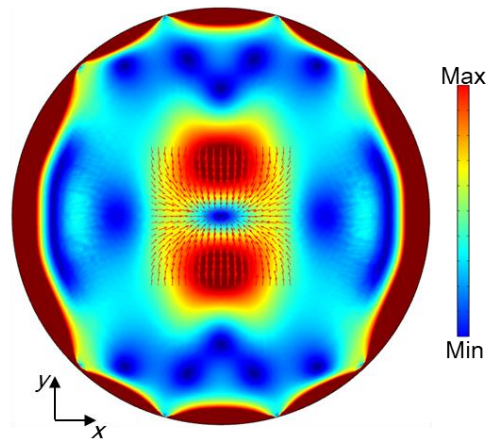


**fig. S3. Simulated acoustic radiation force fields at different frequencies.** (A) Simulation result at 163 kHz. (B) Simulation result at 141 kHz. For these simulations, 10- $\mu\text{m}$  polystyrene particles at the droplet-substrate interface were used. The red arrows represent directions of acoustic radiation forces at different locations.



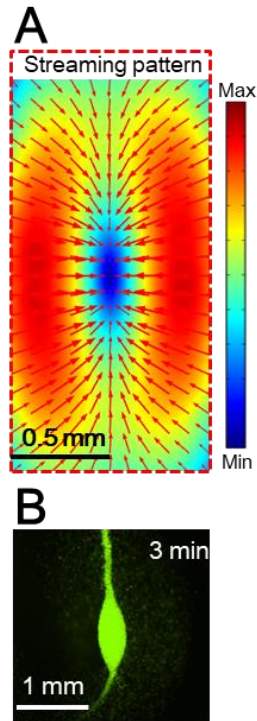
**fig. S4. Simulated flexural wave fields showing the control of in-AFBH nodes.** This simulation employs a 2D cross-sectional model, using an AFBH with an extended bottom diameter  $r_1$  of 6 mm. Perfectly matched layers (PMLs) were placed at the left and right ends to eliminate reflections from substrate ends. The excitation frequency was 147 kHz. To generate pure flexural waves, point displacement-based excitations were used (illustrated by red arrows). The excitations applied to the left and right sides ( $u_0 e^{i\varphi}$  and  $u_0 e^{i(\varphi+\Delta\varphi)}$ ) have a phase difference of  $\Delta\varphi$ . Our simulation results show that waves in the AFBH have smaller wavelengths and higher intensities than those in areas outside the AFBH. Moreover, by changing the phase difference (from 0 to  $\pi$ ), our simulation results show the in-AFBH node positions can be shifted.

Acoustic radiation force field at 147 kHz



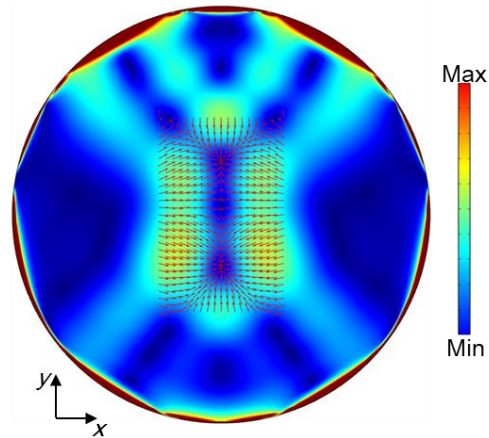
**fig. S5. A simulated acoustic radiation force field for an AFBH between two transducers.** For this simulation, the 10- $\mu\text{m}$  polystyrene particles at the droplet-substrate interface were used. The simulation frequency was 147 kHz. The red arrows represent directions of acoustic radiation forces at different locations.



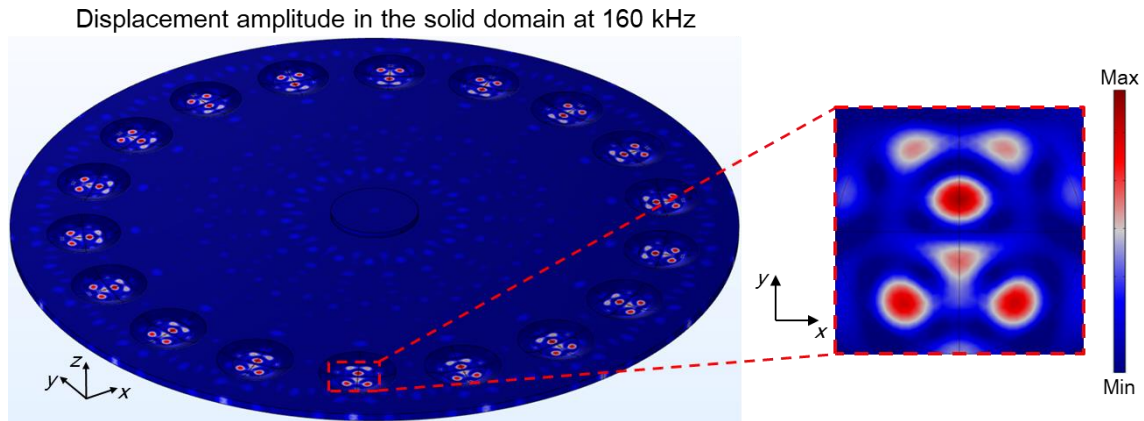


**fig. S6. Simulation and experimental results for the single-site particle enrichment using our device.** (A) A simulation result showing the acoustic streaming pattern around the enrichment area. (B) An acquired microscopy image showing that particles can be enriched by acoustic waves.

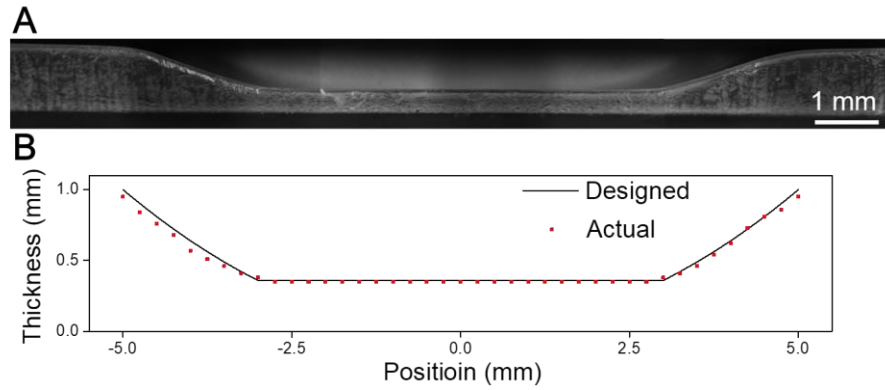
Acoustic radiation force field at 157 kHz



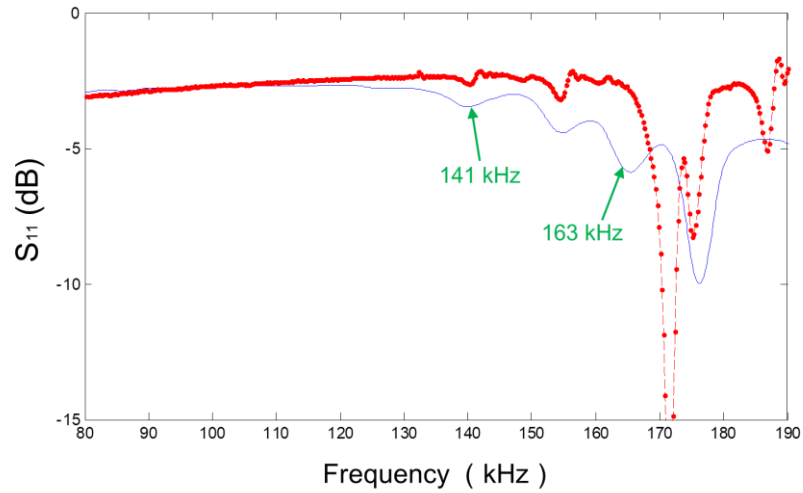
**fig. S7. A simulated acoustic radiation force field for an AFBH of a circular AFBH array.** For this simulation, the 10- $\mu\text{m}$  polystyrene particles at the droplet-substrate interface were used. The simulation frequency was 157 kHz. The red arrows represent directions of acoustic radiation forces at different locations.



**fig. S8. A simulated out-of-plane displacement amplitude field for flexural waves trapped by an array of 18 AFBHs.** The simulation frequency was 160 kHz. This result indicates that our approach can trap flexural waves in multiple AFBHs. Moreover, the mode shapes in individual AFBHs are nearly the same suggesting our approach could potentially be used for high-throughput applications.



**fig. S9. Material thickness characterization results for a PMMA substrate with an AFBH. (A)** A captured cross-sectional image of a PMMA substrate with an AFBH. **(B)** Comparison between the wall profile of the fabricated substrate and the designed profile based on Eq. (1). From the comparison, it can found that the thickness errors are less than 70  $\mu\text{m}$ .



**fig. S10. Reflection coefficient  $S_{11}$  curves for piezoelectric transducers.** We measured the  $S_{11}$  curves for a free piezoelectric transducer (red dotted line) as well as a piezoelectric transducer bonded on an elliptical PMMA substrate (blue solid line) using a vector network analyzer (E5063A, Keysight). The  $S_{11}$  curve for a piezoelectric transducer bonded on an elliptical PMMA substrate shows multiple dips, including two dips near 141 kHz and 163 kHz.

**table S1. Geometrical parameters for an AFBH.**

$h_1$	0.36 mm
$r_1$	3 mm
$a$	$0.04 \text{ mm}^{-1}$
$m$	2
$r_2$	5 mm

**table S2. Material properties used for numerical simulations.**

<b>Water</b>	
Density	$998.2 \text{ kg/m}^3$
Sound speed	1480 m/s
Dynamic viscosity	$1.01 \times 10^{-3} \text{ Pa}\cdot\text{s}$
Bulk viscosity	$2.82 \times 10^{-3} \text{ Pa}\cdot\text{s}$
<b>Polystyrene particles</b>	
Density	$1050 \text{ kg/m}^3$
Sound speed	2350 m/s
<b>PMMA plate</b>	
Density	$1190 \text{ kg/m}^3$
Young's modulus	3.2 GPa
Poisson's ratio	0.35
Isotropic loss factor	0.02
<b>Epoxy</b>	
Density	$1673 \text{ kg/m}^3$
Young's modulus	1 GPa
Poisson's ratio	0.38
Isotropic loss factor	0.02

## **Legends for movies S1 to S3**

**movie S1. AFBH-based arrangement of 10- $\mu\text{m}$  polystyrene particles at two antinodes in an AFBH.** The experiment was performed using an AFBH-based elliptical-substrate device at a frequency of 163 kHz.

**movie S2. AFBH-based arrangement of 10- $\mu\text{m}$  polystyrene particles at three antinodes in an AFBH.** The experiment was performed using an AFBH-based elliptical-substrate device at a frequency of 141 kHz.

**movie S3. AFBH-based enrichment of 10- $\mu\text{m}$  polystyrene particles at an antinode in an AFBH.** The experiment was performed using a setup with an AFBH located between two circular piezoelectric transducers with the same excitation frequency of 147 kHz.

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