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## Supplementary Materials for

### **Optical selection and sorting of nanoparticles according to quantum mechanical properties**

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#### **The PDF file includes:**

Figs. S1 to S4  
Legend for movie S1

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

(available at [advances.sciencemag.org/cgi/content/full/7/3/eabd9551/DC1](https://advances.sciencemag.org/cgi/content/full/7/3/eabd9551/DC1))

Movie S1

## Trajectory analysis of particle motions

We analyzed the trajectories of the particle positions by using an image processing software. Figure S1 represents the trajectory analyzed for the sequential images of an r-ND (Fig. 2A). The trajectory curve is well fitted with a straight line such that the velocity of the particle motion is determined to be  $110 \mu\text{m/s}$ . Figure S2 shows the trajectories of four NDs in the selection and sorting experiment (Fig. 3 and Movie S1). The r-NDs (blue curves numbered 1 and 4) move to the right (direction of GR laser propagation), whereas the n-NDs (pink curves numbered 2 and 3) move in the opposite direction. The differences of the velocities between particles 1 and 4 and between particles 2 and 3 can be ascribed to the differences in the sizes and number of the NVCs. The small deviation of the velocities of NDs is due to the thermally induced random motion of the nanoparticles.

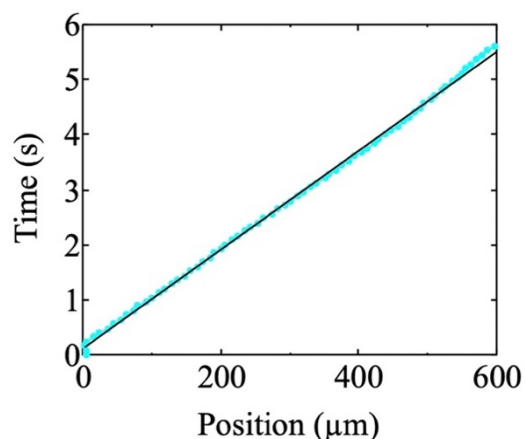


Fig. S1. Trajectory analysis for the transportation of a single r-ND (Fig. 2A).

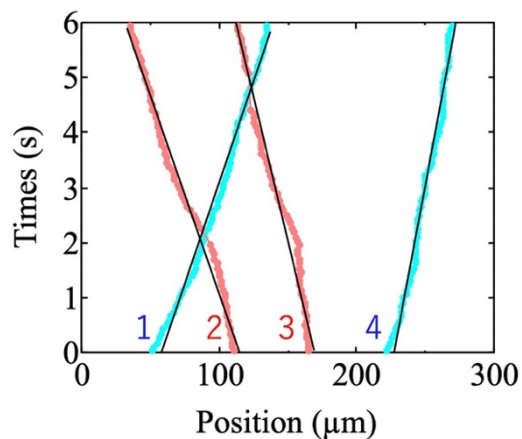


Fig. S2. Trajectory analysis for the selective transportation of r-NDs and n-NDs (Fig. 3).

### Motion control experiment for a single n-ND

We observed the motion control of a single n-ND, where the NIR laser with the power of 250 mW was incident from the right end of the fiber and the power of the GR laser incident from the opposite end was changed from 70 to 0 mW. These experimental conditions are same as that for an r-ND (Fig. 2B). Fig. S3 shows time-sequential images of the n-ND observed at 4 s interval. At the GR laser power of 70 mW, the particle moves from left to right, and the motion decelerates as the GR laser power decreases, and then the r-ND moves toward the opposite direction.

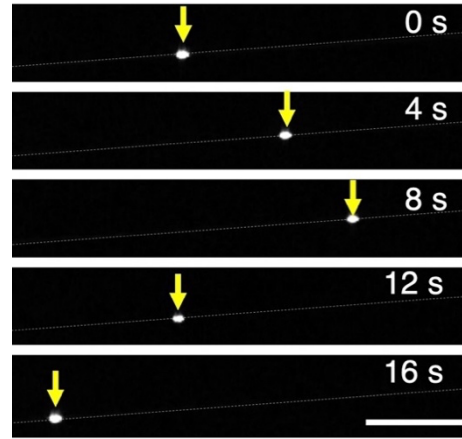


Fig. S3. Motion control of a single n-ND along a nanofiber  
The white bar indicates a scale of 100  $\mu\text{m}$ . The dotted line represents the nanofiber position.

### Refractive indices of the nanodiamond and water

In the calculation of the scattering cross-sections for the analysis without reference particles (see Materials and Methods section), we used the different values of the refractive indices at the different wavelengths for the nanodiamond ( $n = 2.425$  at 532 nm,  $n = 2.393$  at 1064 nm) and water ( $n = 1.334$  at 532 nm,  $n = 1.326$  at 1064 nm).

### Determination of the distance between a nanoparticle and the nanofiber

We determine the distance between a particle and the nanofiber by the optical trapping potential and thermodynamic analyses. The particle is attracted towards the fiber surface by the optical gradient force of the evanescent field around the fiber. The trapping potential of this gradient force is given by

$$U(d) = \frac{1}{2} \alpha |E_0|^2 \exp\left(-\frac{d}{\gamma}\right)$$

where  $\alpha$  is the polarizability of the nanoparticle,  $E_0$  is the electric field at the center of the particle when it is in contact with the fiber,  $\gamma$  is the penetration depth of the evanescent field, and  $d$  is the distance between facing surfaces of the particle and fiber. Under the thermal equilibrium condition, the average distance  $d$  is determined from  $U(d) = kT$ , where  $k$  is the Boltzmann constant and  $T$  is the room temperature. The estimated average distance for the absorption cross-section analysis is 5.1 nm.

### Determination of the optical force exerted on a single ND

We determine the optical force from the velocity of the particle motion based on the balance with the viscous drag. The viscous drag force exerted on the particle near the surface is given by the Faxen formula (23), as follows,

$$F = 6\pi\mu r v \left\{ 1 - \frac{9}{16} \left( \frac{r}{r+d} \right) + \frac{1}{8} \left( \frac{r}{r+d} \right)^3 - \frac{45}{256} \left( \frac{r}{r+d} \right)^4 - \frac{1}{16} \left( \frac{r}{r+d} \right)^5 \right\}^{-1}$$

where  $\mu$  is the viscosity of the medium,  $r$  and  $v$  are the radius and velocity of the particle, respectively, and  $d$  is the distance between the facing surfaces of the particle and fiber. In the measurement, we selected NDs with approximately the same scattering intensity around the average, such that the size deviation can be reduced. Thus, we set the particle radius to 25 nm (from the datasheet), and the distance  $d$  is 5.1 nm as mentioned above.

### Distribution of the absorption cross-sections for r-NDs

The absorption cross-section evaluated for ten r-NDs is  $3.3 \pm 1.1 \times 10^{-14} \text{ cm}^2$ . Their distribution is shown as a histogram in Fig. S4.

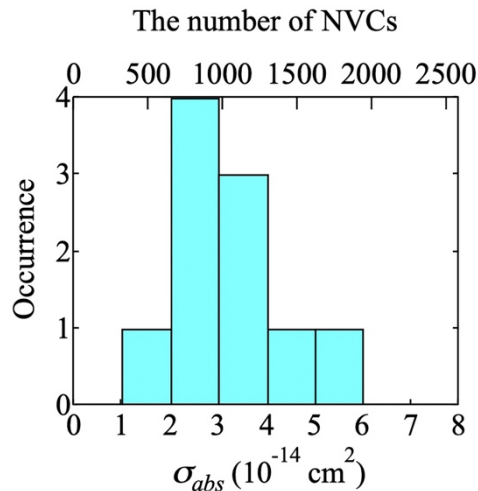


Fig. S4. Distribution of the absorption cross-sections evaluated for ten r-NDs.

### **Estimation of the number of NVCs for r-NDs**

When the absorption cross-section  $\sigma_{abs}$  of a single NVC is known, the number of NVCs in a single r-ND can be determined. By using the reported value of  $\sigma_{abs}$  for a single NVC ( $3.1 \times 10^{-17} \text{ cm}^2$ ; Ref. 28), the average  $\sigma_{abs}$  of r-NDs ( $3.3 \times 10^{-14} \text{ cm}^2$ ) evaluated in the experiment corresponds to 1060 NVCs. In Fig. S4, the number of NVCs in individual NDs is scaled on the upper axis.

### **Movie S1.**

Selective transportation of r-NDs and n-NDs using counter-propagating GR and NIR lasers. Particles 1 and 4 represent r-NDs and particles 2 and 3 represent n-NDs, which is confirmed by the emission from the NVCs. The powers of GR and NIR lasers were set as 7.40 mW and 160 mW, respectively. The r-NDs move to the right (direction of GR laser propagation), whereas the n-NDs move in the opposite direction.