Electronic Supplementary Material (ESI) for Analyst.

Supplementary information

Shape Characterization and Discrimination of Single Nanoparticles using Solid-state Nanopores

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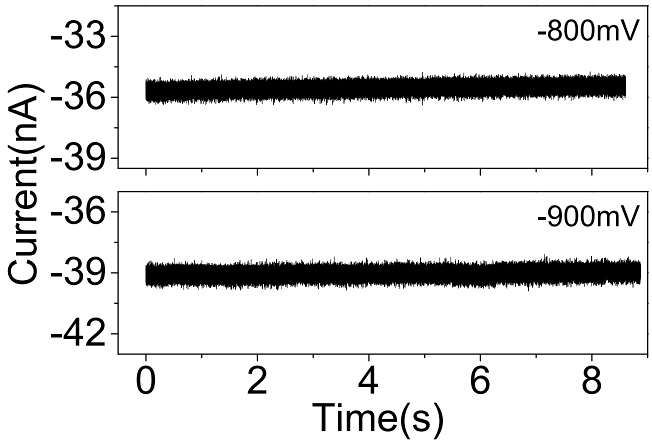

Figure S1. Open pore current trace *versus* time when no nanoparticles were added to the chambers.

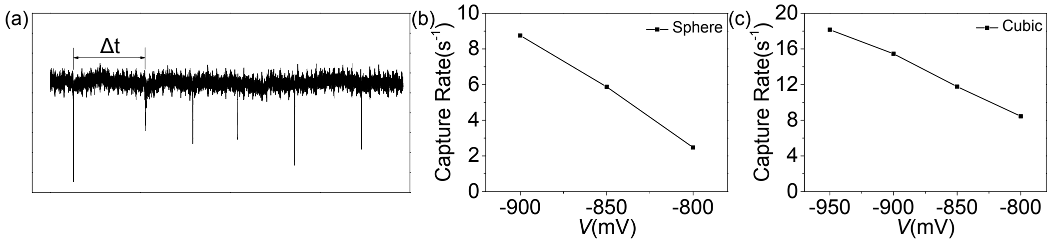

Figure S2. Capture rate calculation for the nanoparticles translocating through nanopores. (a) An ionic current trace *versus* time when nanoparticles were translocating through the nanopore. Δt indicates the time intervals between two adjacent current blockades. The capture rate was then calculated as $1/\Delta t$. (b) The relationship between the capture rate and the applied bias voltage for the spherical nanoparticles. (c) Same as panel b but for the cubic nanoparticles.

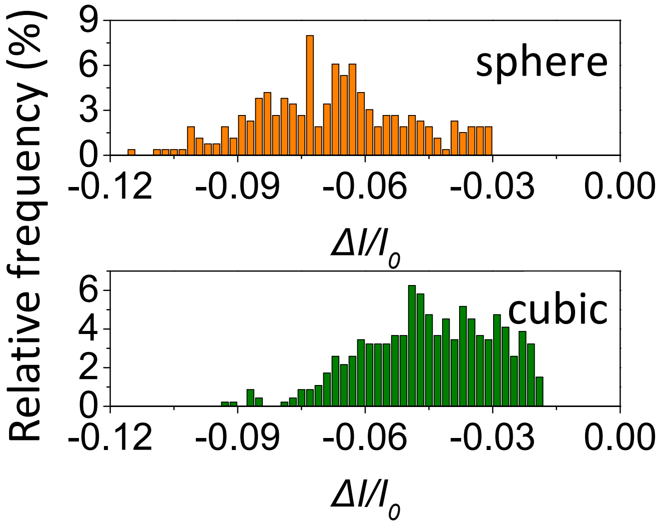

Figure S3. The relative frequency distribution histograms of relative current blockade for the spherical (above) and cubic (below) nanoparticles. All the data were measured at a bias voltage of -850 mV. Only 263 and 464 events from 30-second current traces were used to plot the histograms for spherical and cubic nanoparticles, respectively.

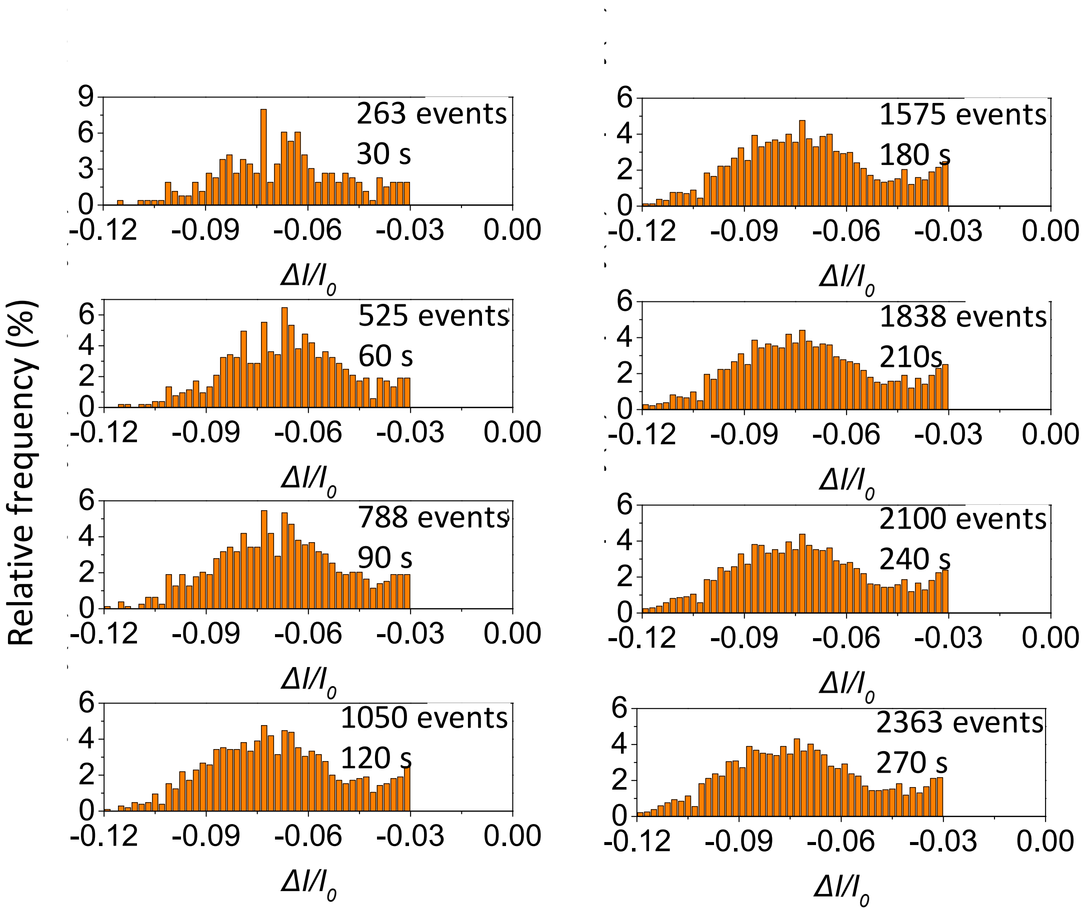

Figure S4. The relative frequency distribution histograms of relative current blockade for the spherical nanoparticles. All the data were measured at a bias voltage of -850 mV. The number of events and the duration of current traces were put as inserts in each panel.

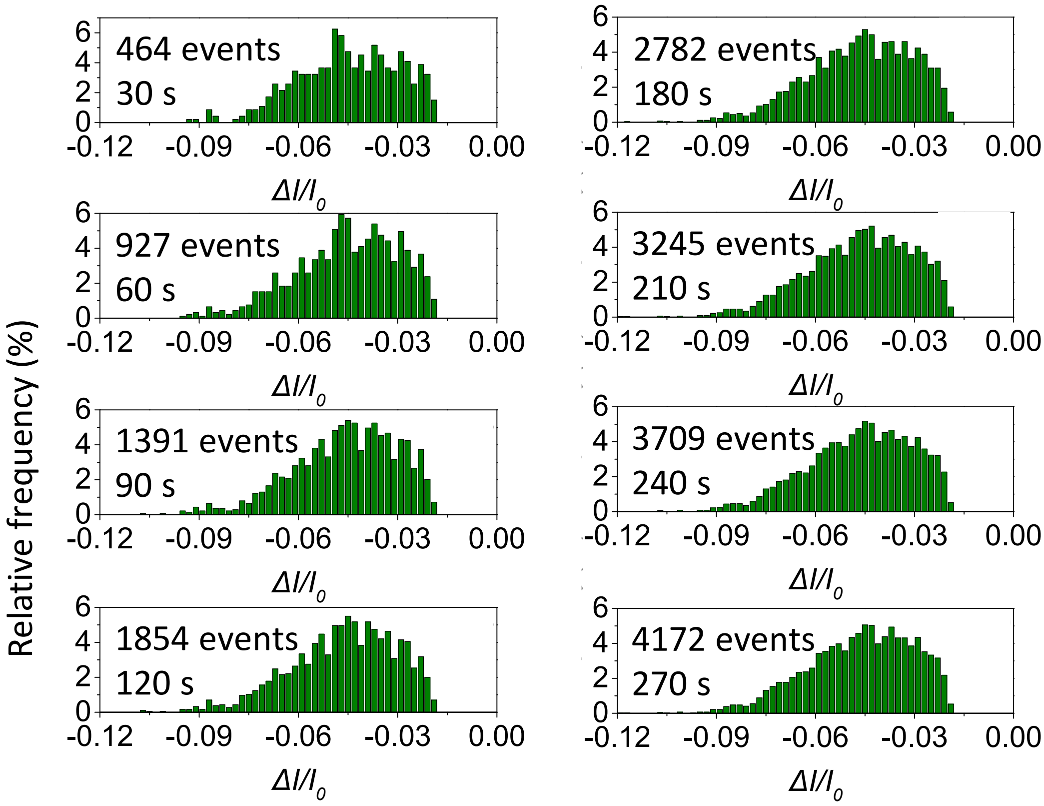

Figure S5. The relative frequency distribution histograms of relative current blockade for the cubic nanoparticles. All the data were measured at a bias voltage of -850 mV. The number of events and the duration of current traces were put as inserts in each panel.

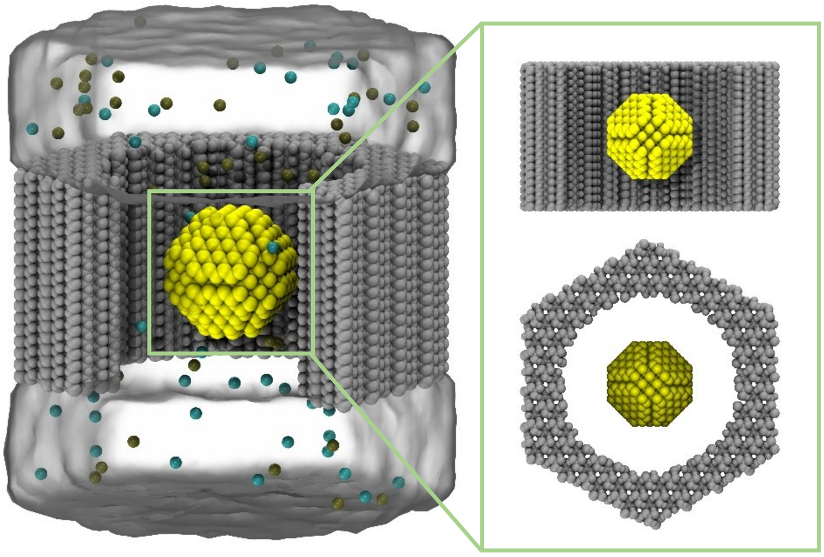

Figure S6. The illustration of the simulation setup of a spherical nanoparticle in the nanopore.

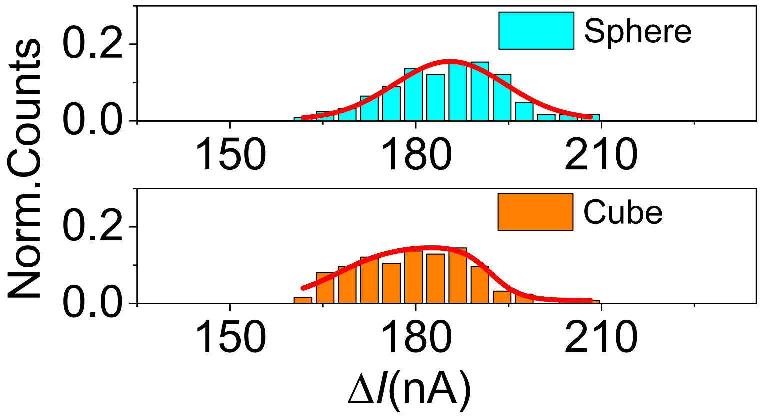

Figure S7. The frequency histograms of the current blockade for the spherical (above) and cubic (below) nanoparticles. The data were analyzed based on 10-ns long production simulations. The red solid lines for the spherical and cubic nanoparticles are the fitted lines by using the standard Gaussian distribution function and the unsymmetrical peak function (equation (2) in the main text), respectively.

Supplementary Method: The differential hash algorithm (DHA) was adopted to analyze and compare the histograms of the current blockade obtained from the experiments and simulations. DHA is a generic term for a class of comparative hash methods. The features contained in the histograms are used to generate a set of fingerprints (though it is probably not unique), which can be used for further comparison between them. Below are the simple steps we used to compare the results from experiments and simulations. We firstly zoomed out the histograms from both the experiments and simulations to remove high frequencies and details but preserve the light and shade of the structure. The plots were finally reduced to 9×8 grids (72 pixels in total) to eliminate structure differences in different sizes and proportions and make the effect of bin size negligible. Secondly, the colorful histograms were converted to histograms with a 64-level grayscale to simplify the color, meaning all pixels have only 64 colors. Thirdly, we calculated the viarance value, each row of the matrix was performed as follows: the two adjacent elements were subtracted (the left element minus the right element) to produce 8 different variance values, resulting 64 variance values in total. Fourthly, the variance values were processed, which were remembered as 1 if it is positive or 0, or 0 if it is negative. Finally, by combining 64 results we could obtain a hash value (the 64 values in each histogram are in the same order), which is the "fingerprint" of the histogram and then compare the similarity between the histograms. By using this algorithm, we obtained 93.24% similarity between the histograms for the cubic nanoparticles shown in Figure 4b and Figure 5c. Analogously, we also got 93.24% and 93.72% similarities for only the fitted lines and the histograms combined with the fitted lines, respectively. These results further validate that the shape of the histograms of current blockade from our simulations actually fit the data from experiments.

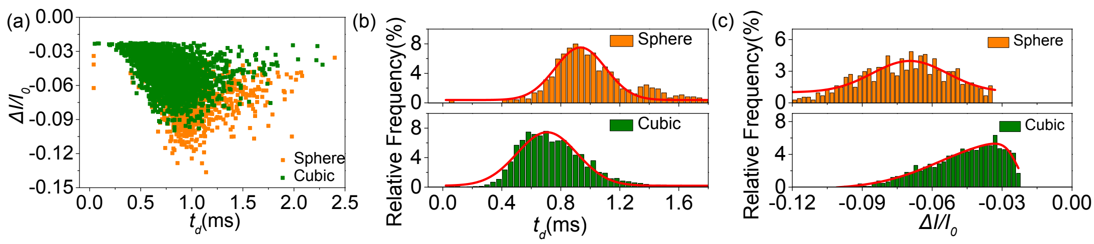

Figure S8. Characterization and differentiation of spherical and cubic nanoparticles by current signals. (a) Scatter plots of two different-shaped nanoparticles. Yellow and green symbols are for spherical and cubic nanoparticles, respectively. (b) The comparison between the frequency distribution histograms of duration for the spherical and cubic nanoparticles. The red solid lines are the fitted lines by using the standard Gaussian distribution functions. (c) Same as panel b but for the frequency distribution histograms of relative current blockade. The red solid lines in panel c for the spherical and cubic nanoparticles are the fitted lines by using the standard Gaussian distribution function and the unsymmetrical peak function, respectively. All the data were measured at a bias voltage at -800 mV.

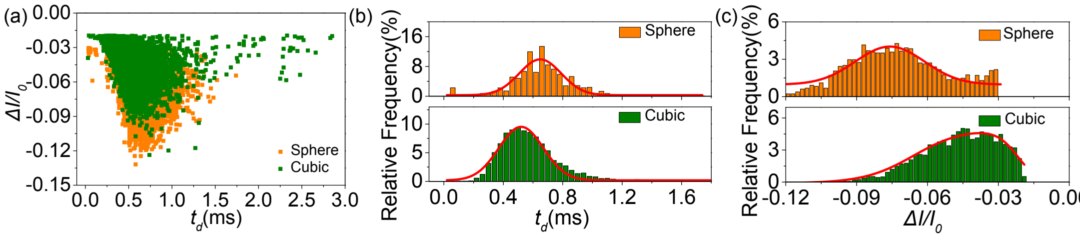

Figure S9. Characterization and differentiation of spherical and cubic nanoparticles by current signals. (a) Scatter plots of two different-shaped nanoparticles. Yellow and green symbols are for spherical and cubic nanoparticles, respectively. (b) The comparison between the frequency distribution histograms of duration for the spherical and cubic nanoparticles. The red solid lines are the fitted lines by using the standard Gaussian distribution functions. (c) Same as panel b but for the frequency distribution histograms of relative current blockade. The red solid lines in panel c for the spherical and cubic nanoparticles are the fitted lines by using the standard Gaussian distribution function and the unsymmetrical peak function, respectively. All the data were measured at a bias voltage at -900 mV.