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Supporting information for article:

Scattering Functions of Carved Ellipsoid-Shaped Particles

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Fitting process of experimental curve in the text.

Due to the limitation of computing power, we were unable to fit all 5 parameters at the same time. Therefore, according to the shape of $\{Mo_{154}\}$ from single crystal data, we fixed 3 parameters, $a = 17.5$ Å, $c = 9.0$ Å, $\alpha = 0.66$, to explore the influence of b and r_0 and the best fitting result in this condition. To evaluate the goodness of fit, we introduced a criterion

$$\frac{1}{Var} = \frac{1}{\Delta p_1^2 + \Delta p_2^2 + \Delta p_3^2}$$

in which Δp means the q value difference between the corresponding peaks of experimental curve and model curve. The larger $\frac{1}{Var}$ is, the better the fitting is. From Figure S2, $b = 14$ Å, $r_0 = 0.76$ gave the best result.

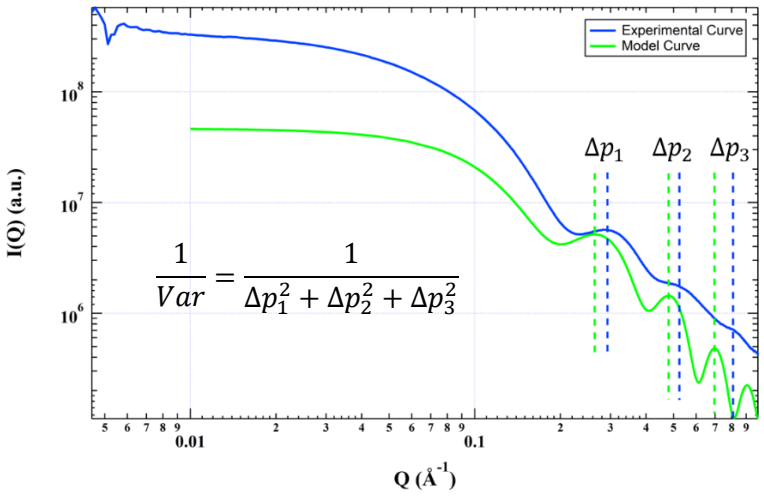

Figure S1. The criterion $\frac{1}{Var}$ to evaluate the goodness of fit. Blue curve: experimental curve; Green curve: model curve.

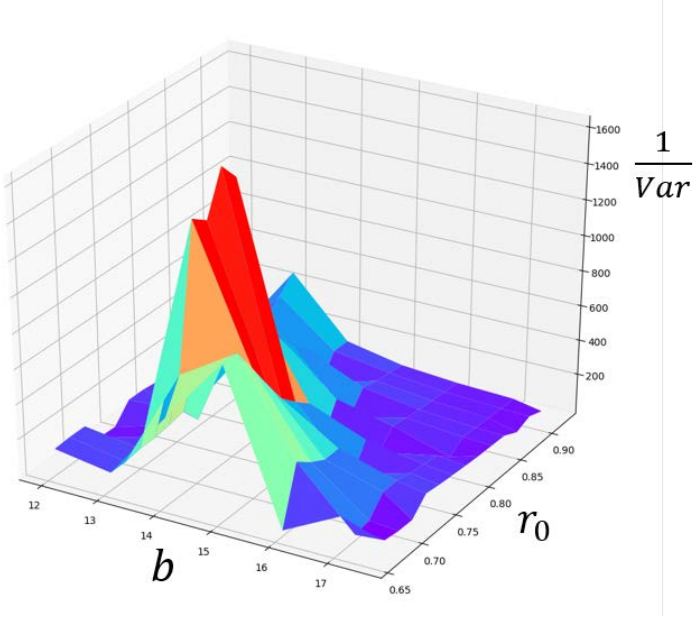

Figure S2. The influence of b and r_0 and the determination of the best fitting result.

Two more fitting examples of custom carved ellipsoid model

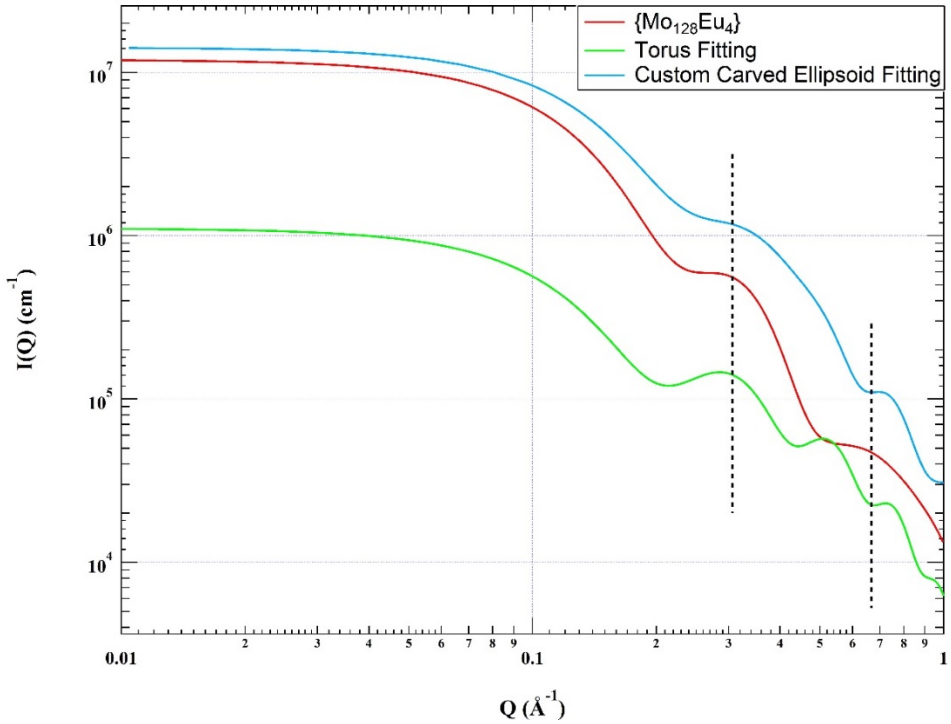

Figure S3. Fitting results of $\{Mo_{128}Eu_4\}$. red curve: theoretical curve of $\{Mo_{128}Eu_4\}$; green curve: torus model fitting curve; blue curve: custom carved ellipsoid model fitting curve.

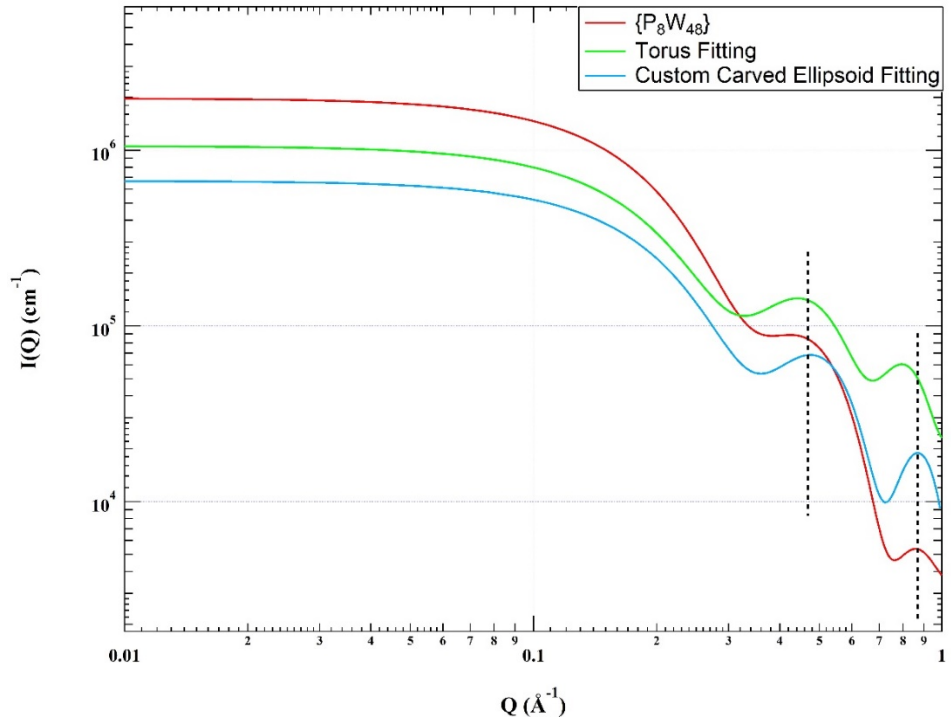

Figure S4. Fitting results of $\{P_8W_{48}\}$. red curve: theoretical curve of $\{P_8W_{48}\}$; green curve: torus model fitting curve; blue curve: custom carved ellipsoid model fitting curve.