Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

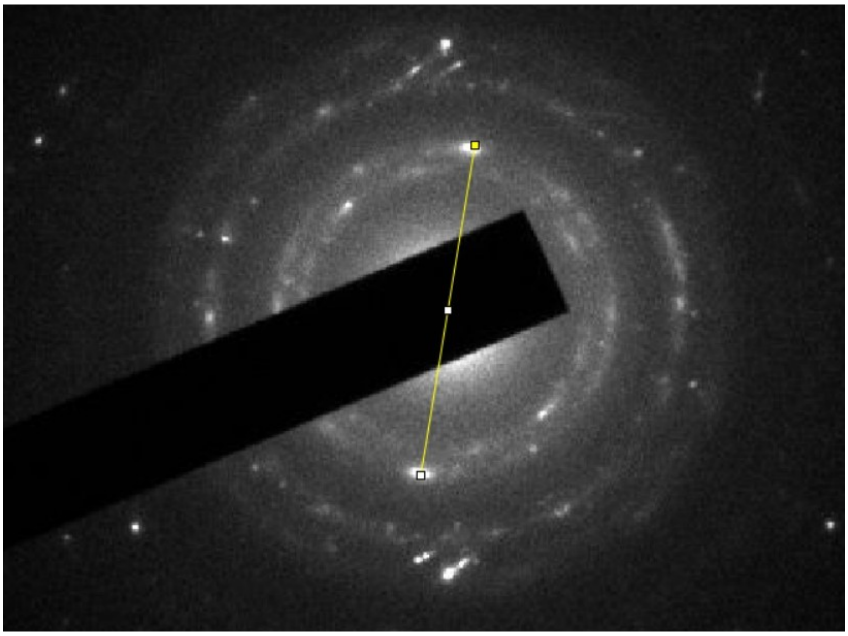
Electronic Supplementary Information

Investigation of Enhanced Third-Order Optical Nonlinearity in Novel Coenzyme-A Capped Silver Nanoparticles

Aditya Dileep Kurdekar[#1,2], Prajal Chettri[#2], Rajasimha Kurnoothala[2], Chelli Sai Manohar[3], Shailesh Srivastava[2], Krishna Chaitanya Vishnubhatla[2]

S1. Estimation of Lattice planes of silver nanoparticles based on TEM-SAED pattern

By using Image J software, we calculated the diameter of the 4 rings as followed in Table as Lengths. These values may vary depending on the taken set scale, but the ratios will come always same.



Results

File Edit Font Results

	Area	Mean	Min	Max	Angle	Length
1	135	74.186	0.802	255.000	-47.411	134.469
2	157	72.232	0.000	254.944	-98.858	155.859
3	222	76.548	0.000	238.790	-59.482	220.554
4	259	80.780	0.000	255.000	-90.000	258.000

From the figure it appears that the first two rings were closer followed by 3rd and 4th were closer indicating a FCC pattern.

For cubic crystals, $d_{hkl} = a_0/(h^2+k^2+l^2)^{1/2}$ where d_{hkl} is the d spacing, a_0 is the lattice constant, h,k & l are the Miller indices.

Using the equivalence of D spacing and radium of rings,

$R_{hkl} = (\lambda L/a_0)(h^2+k^2+l^2)^{1/2}$

As the value of $(\lambda L/a_0)$ is constant for a given diffraction pattern, the values of R_{hkl} vary according to $(h^2+k^2+l^2)^{1/2}$.

By using the ratios:

$R_1/R_2 = d_1/d_2 = (h_1^2+k_1^2+l_1^2)^{1/2} /(h_2^2+k_2^2+l_2^2)^{1/2} = 134.469/155.859= 0.862$

$R_2/R_3 = d_2/d_3 = (h_2^2+k_2^2+l_2^2)^{1/2} /(h_3^2+k_3^2+l_3^2)^{1/2} = 155.859/220.554= 0.706$

$R_3/R_4 = d_3/d_4 = (h_3^2+k_3^2+l_3^2)^{1/2} /(h_4^2+k_4^2+l_4^2)^{1/2} = 220.554/258.000= 0.854$

However, the above obtained values are only possible if the planes are {111}, {200}, {220}, {311} as

$R_1/R_2 = 0.862 \sim (1^2+1^2+1^2)^{1/2} /(2^2+0^2+0^2)^{1/2} = 0.866$

$R_2/R_3 = 0.706 \sim (2^2+0^2+0^2)^{1/2} /(2^2+2^2+0^2)^{1/2} = 0.707$

$R_3/R_4 = 0.854 \sim (2^2+2^2+0^2)^{1/2} /(3^2+1^2+1^2)^{1/2} = 0.852$

Thus, we can conclude that allowed reflections are for an fcc crystal lattice. The order of rings in increasing radius are: {111}, {200}, {220}, {311}, {222}, {400}, {331}, {420}, {422} …

Table S1- Third-order non-linear susceptibility $\chi^{(3)}$ of various nanoparticle systems reported in the literature

S.No	Material	Reference	$\chi^{(3)}$ material	$\chi^{(3)}$ standard	Reference
1	AgNPs- CoA in water	CS_2	1.38×10^{-13}	1.75×10^{-12}	Present work
2	AgNPs in water	CS_2	2.95×10^{-14}	-	(45)
3	Ag colloids in acetone	CCL_4	1.89×10^{-14}	4.40×10^{-14}	(52)
4	Ag colloids in DCM	CCL_4	3.6×10^{-12}	4.40×10^{-14}	(52)
5	Ag colloids in chloroform	CCL_4	5.3×10^{-13}	4.40×10^{-14}	(52)
6	AgNPs in water	CS_2	7.7×10^{-14}	9.32×10^{-12}	(53)
7	AuNPs in water	CS_2	5.52×10^{-13}	9.32×10^{-12}	(53)
8	AuNPs in water	CCL_4	1.93×10^{-14}	4.40×10^{-14}	(54)