Electronic Supplementary Material (ESI) for RSC Advances.

APPENDIX

A. Characterization of synthesized borohydride stabilized silver nanoparticles

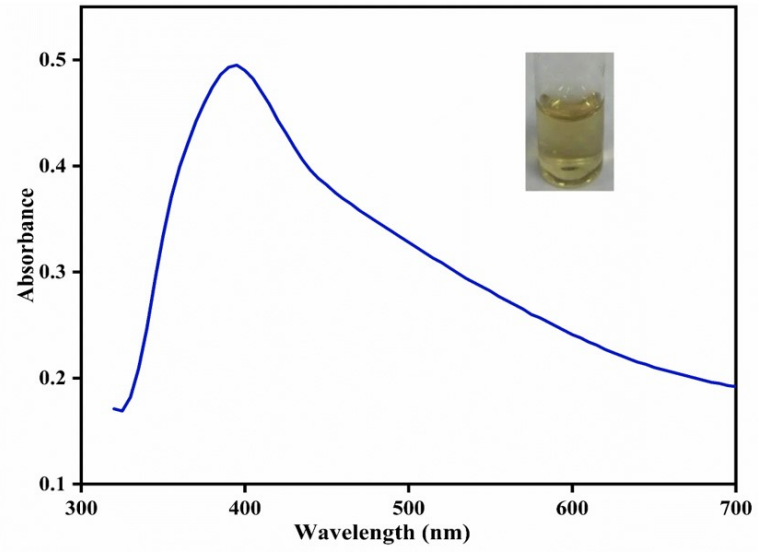
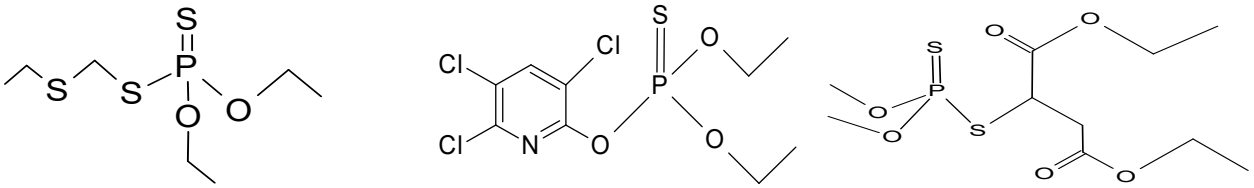


Fig. A.1. The UV-visible absorption spectrum of the colloidal silver nanoparticle synthesized.

Table A.1. Variation of absorbance peak and its intensity of solution containing synthesized silver nanoparticles with time at 4°C and 25°C

Time from Synthesis Day		**0**	**5th Day**	**10th Day**	**15th day**
Storage temperature					
4°C	**λ_{max} (nm)**	390	390	390	395
	Absorbance	0.495	0.493	0.490	0.486
25°C	**λ_{max} (nm)**	390	390	395	395
		0.495	0.473	0.461	0.389

B. Chemical Structure of the pesticides



Phorate **Chlorpyrifos** **Malathion**

C. Color and UV-visible spectra change of NP-Phorate, NP- Chlorpyrifos and NP-Malathion mixture

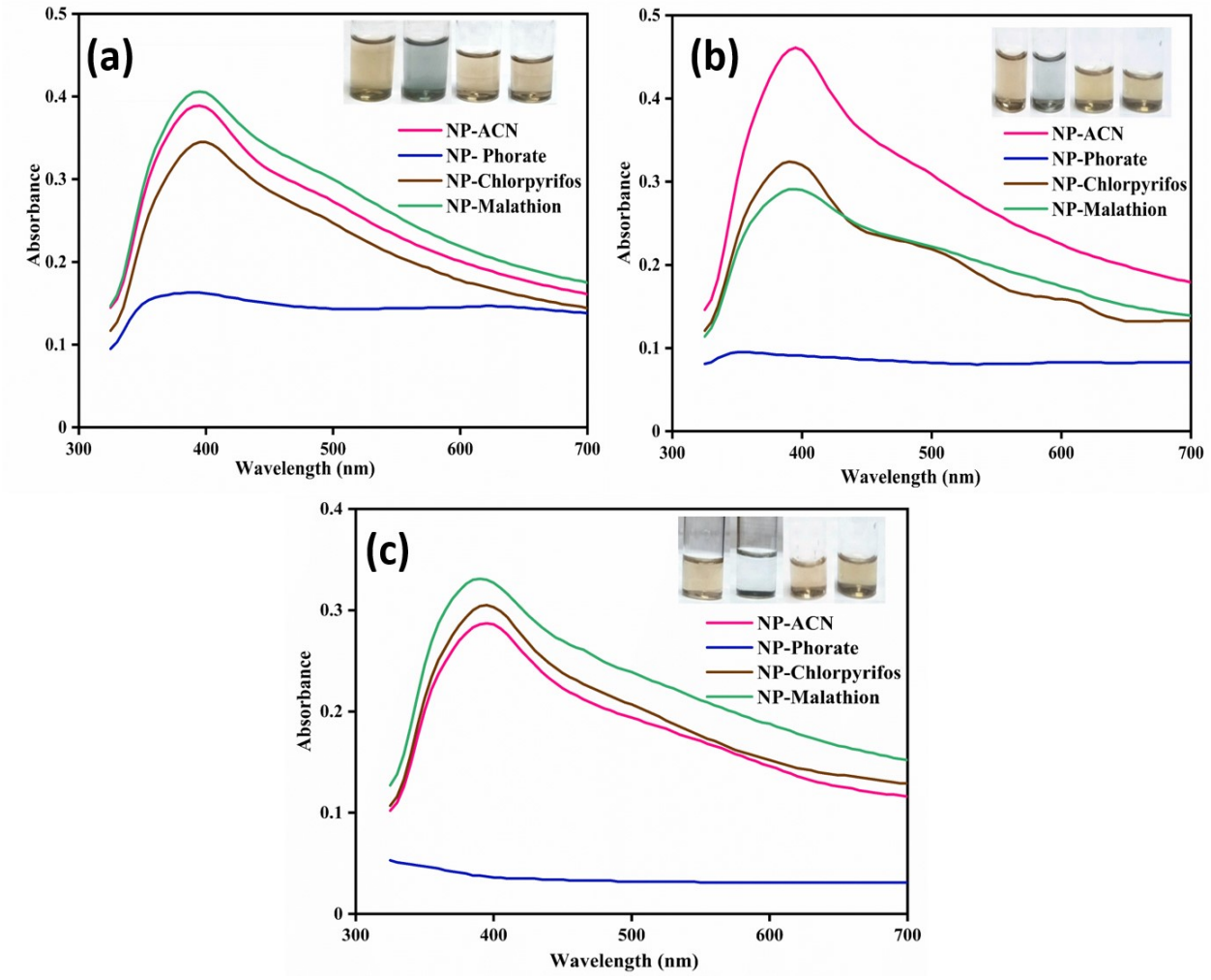


Fig. C.1. Image of color change and corresponding UV-visible spectra change for NP-ACN, NP-Phorate, NP-Chlorpyrifos, and NP-Malathion mixture at (a) half an hour (b) 2 hours and (c) 12 hours of incubation at 4°C

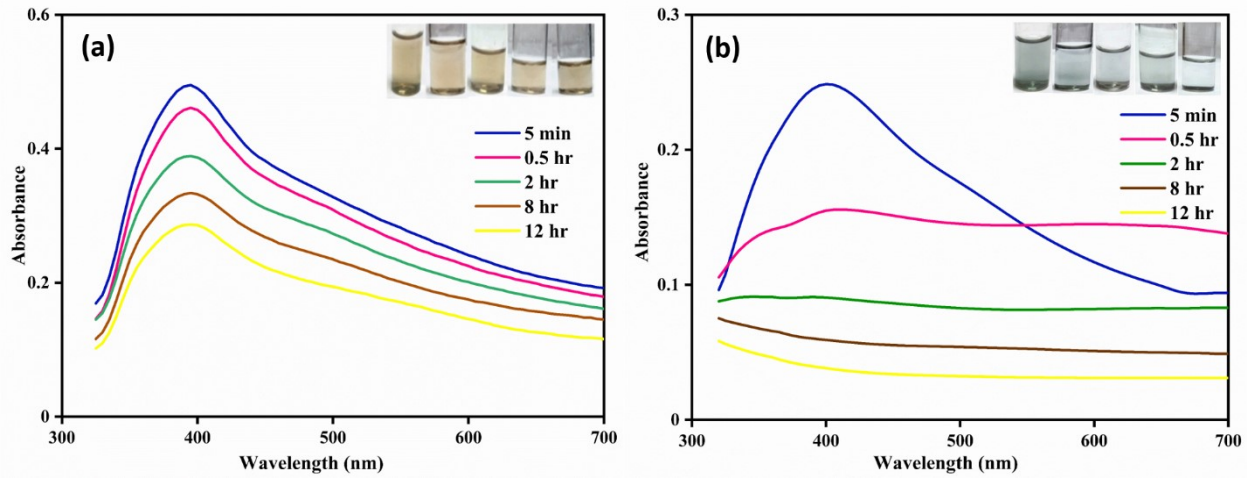


Fig. C.2. Image of color change and corresponding UV-visible spectra change for (a) NP with no phorate and (b) NP-Phorate mixture at 5min, 0.5, 2, 8, 12 hours of incubation along with control sample at 4°C

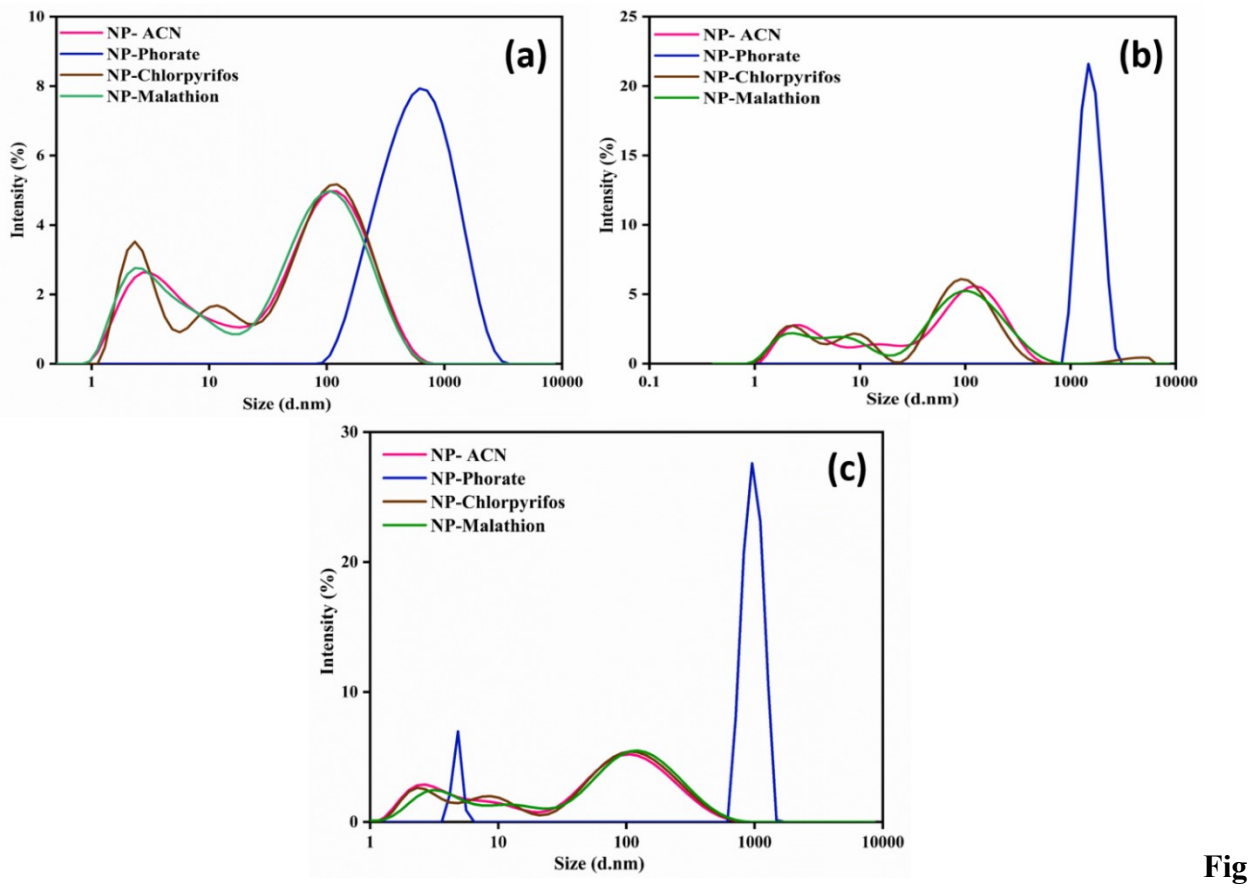


Fig. C.3. Particle size distribution of NP-Phorate, NP- Chlorpyrifos and NP- Malathion mixture at (a) 5min (b) 2 hours and (c) 12 hours of incubation at 4°C

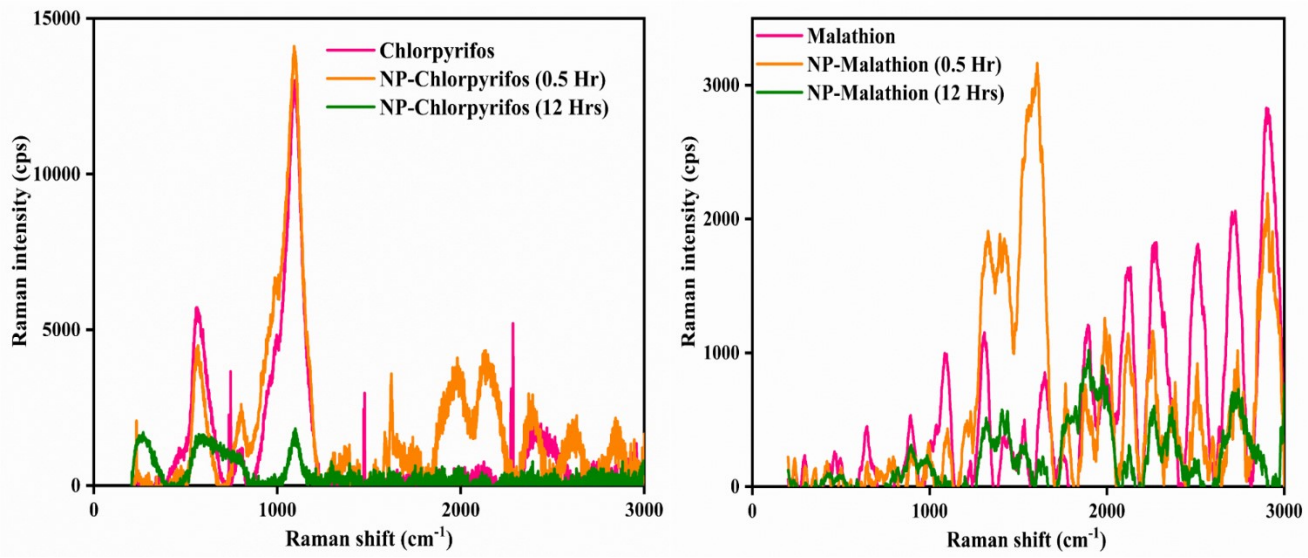
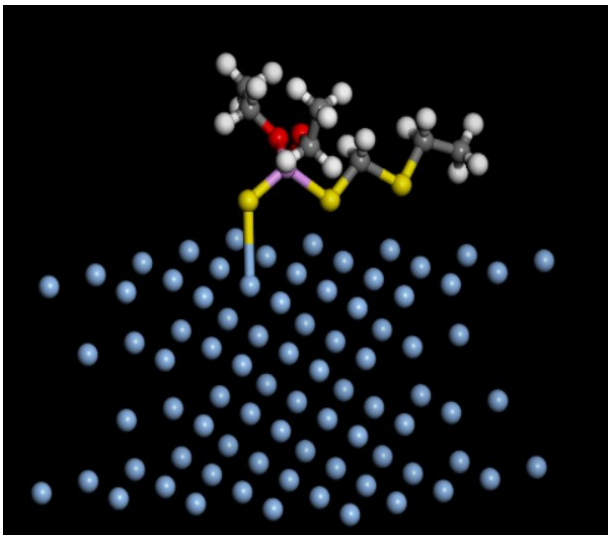
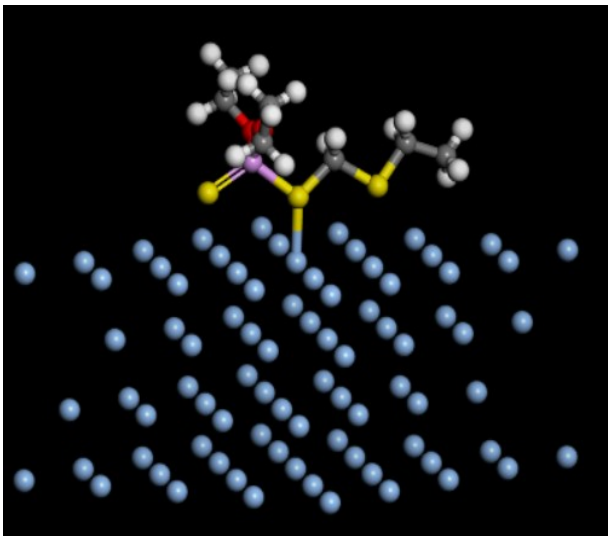


Fig. C.4. Raman spectra of chlorpyrifos, malathion, NP-chlorpyrifos, and NP-malathion mixture at 0.5 hours and after incubation of 12 hours

D. Adsorption energy calculations of phorate molecule on the silver surface – Ag (1 1 1) using DFT simulation

Table D.1. Graphical description of the various configurations for which the adsorption of phorate is studied on the silver surface – Ag (1 1 1)

Bonding Moiety	Adsorption Site	Graphical Description
-P=S	top	
-S- (S1)	top	

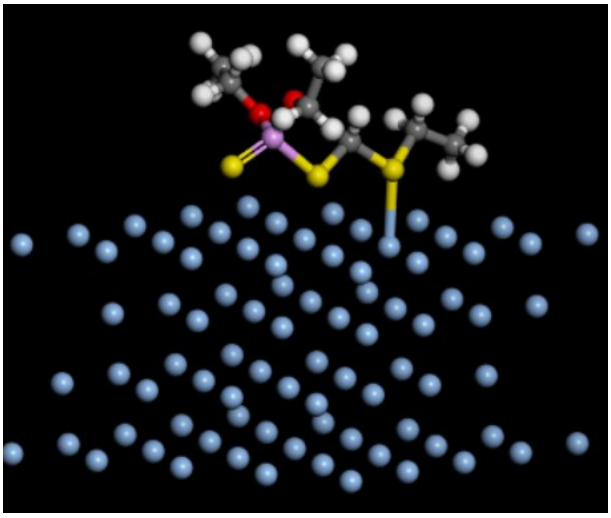
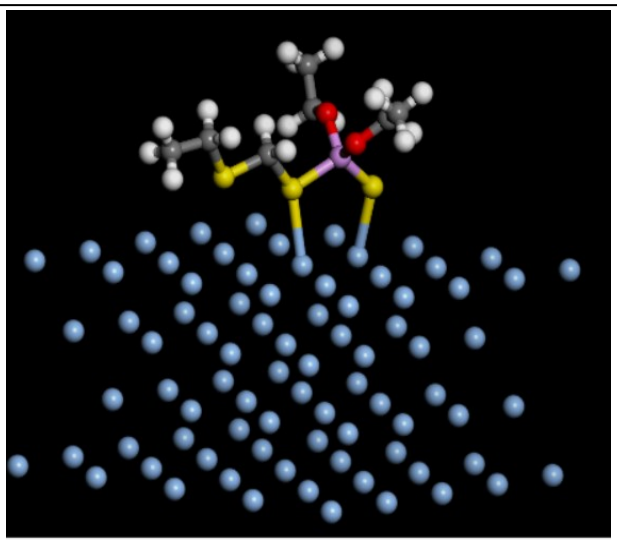
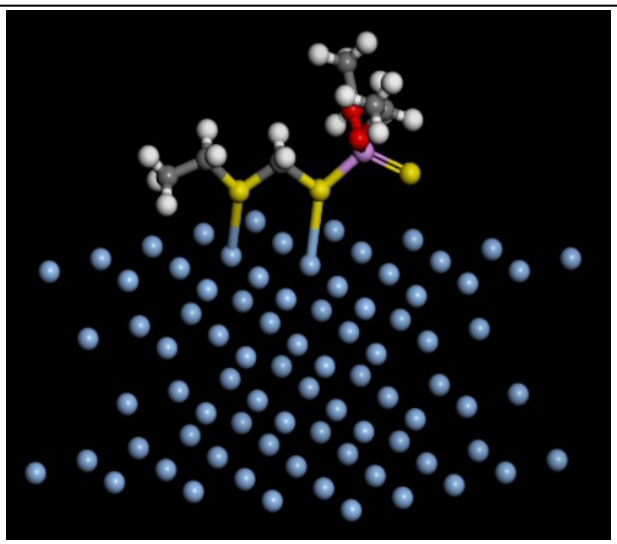
-S- (S2)	top	
-P=S, -S-	top, top	
-S-, -S-	top, top	

Table D.2. The adsorption energy of phorate in various configurations on the silver surface – Ag (1 1 1) (including entropic contributions)

Bonding Moiety	***Adsorption Site***	**Adsorption Energy (kcal/mol)**
-P=S	top	-31.44
-S- (S1)	top	-33.49
-S- (S2)	top	-36.91
-P=S, -S-	top, top	-33.49
-S-, -S-	top, top	-37.46