Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

Rapid nucleation and optimal surface-ligand interaction stabilize Wurtzite MnSe

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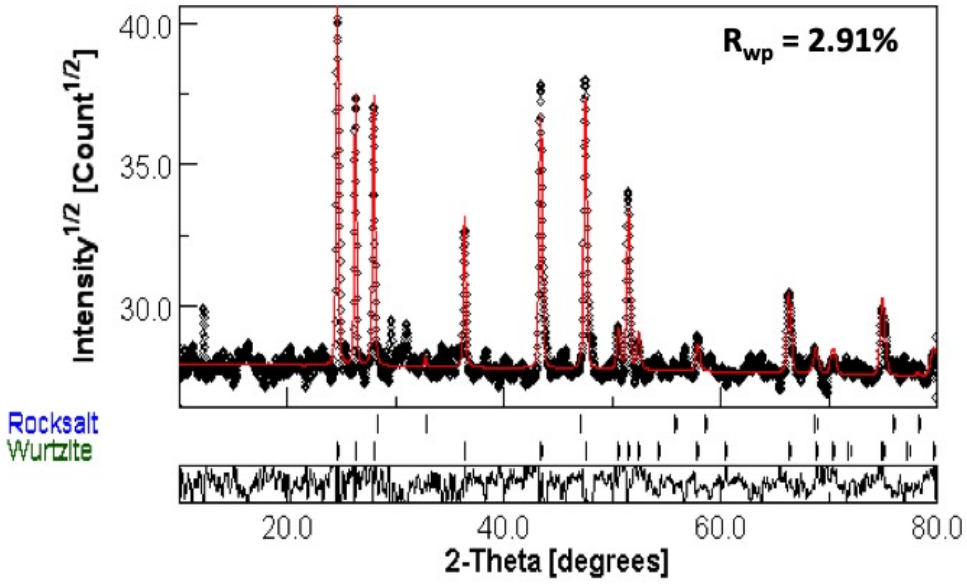


Figure S1. XRD Rietveld Refinement of MnSe Wurtzite Spectra along with the Rocksalt.

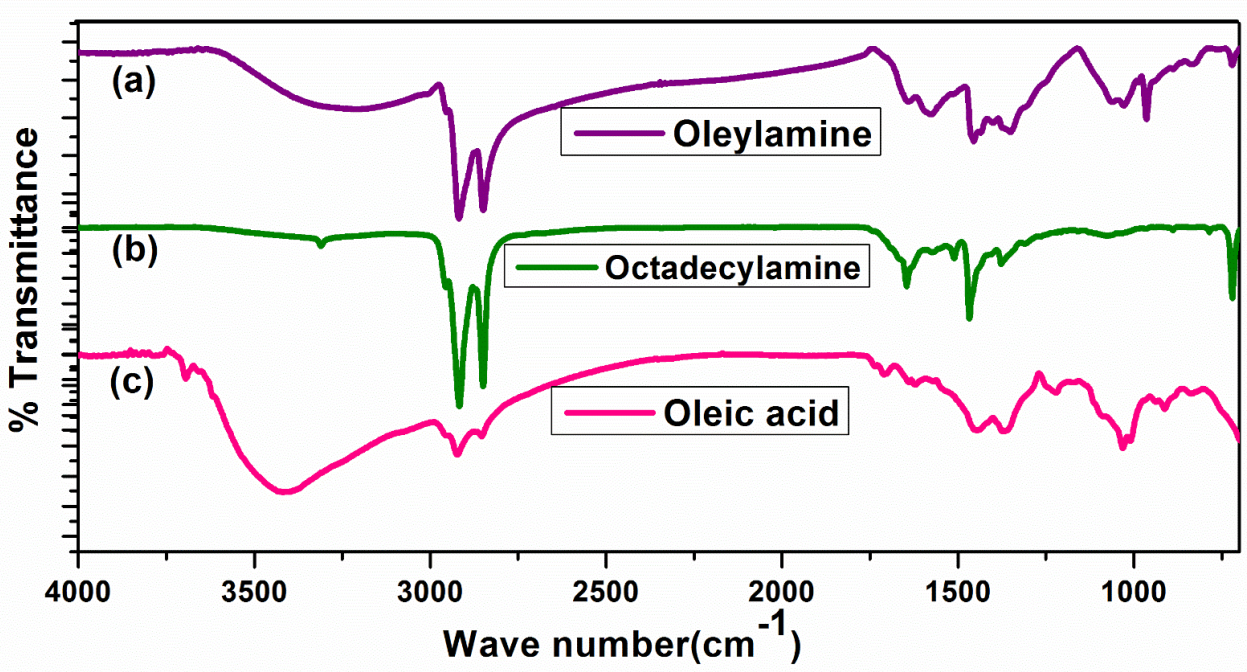


Figure S2. FTIR spectra of (a) Rocksalt phase synthesized with oleylamine, (b) Rocksalt phase synthesized with octadecylamine and c) Wurtzite phase synthesized with oleic acid.

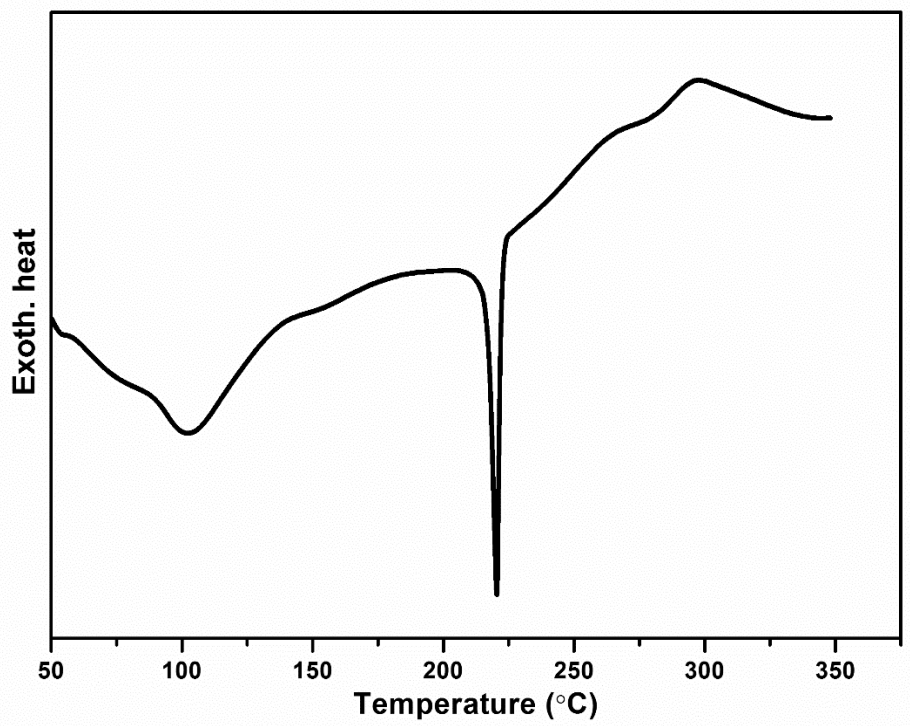
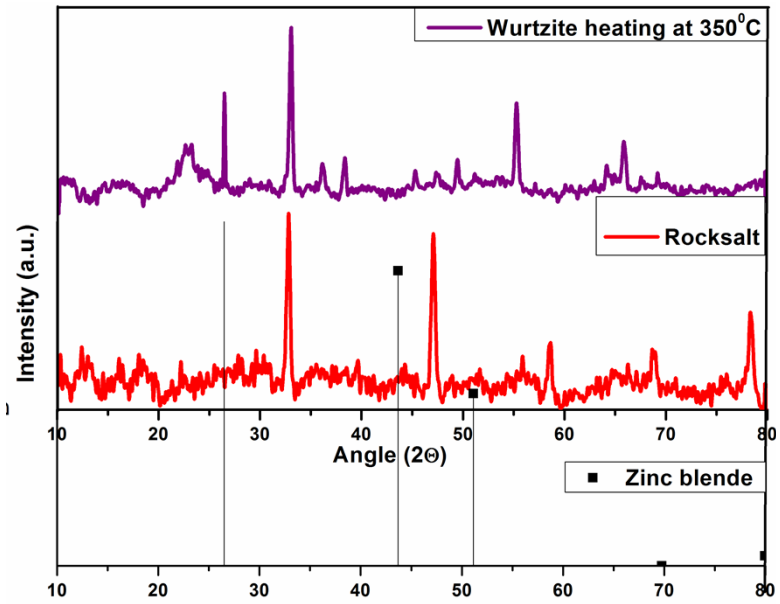


Figure S3. DSC curve of the Wurtzite/NNS.

(a)



(b)

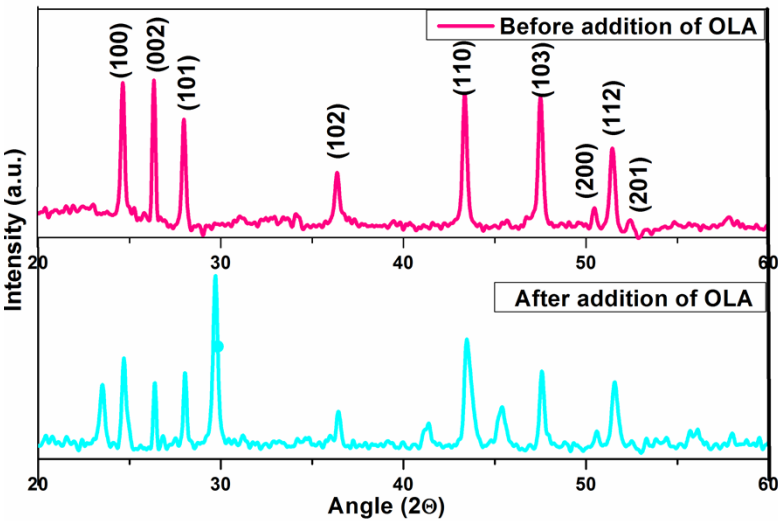


Figure S4. a) XRD pattern (from top to bottom) of Wurtzite along with the rock salt (when Wurtzite heated at 350 ^{0}C) and standard Zinc blende polymorph of MnSe, b) (from top to bottom) XRD of Wurtzite polymorph before and after addition of oleylamine (no phase change observed after ligand exchange reaction).

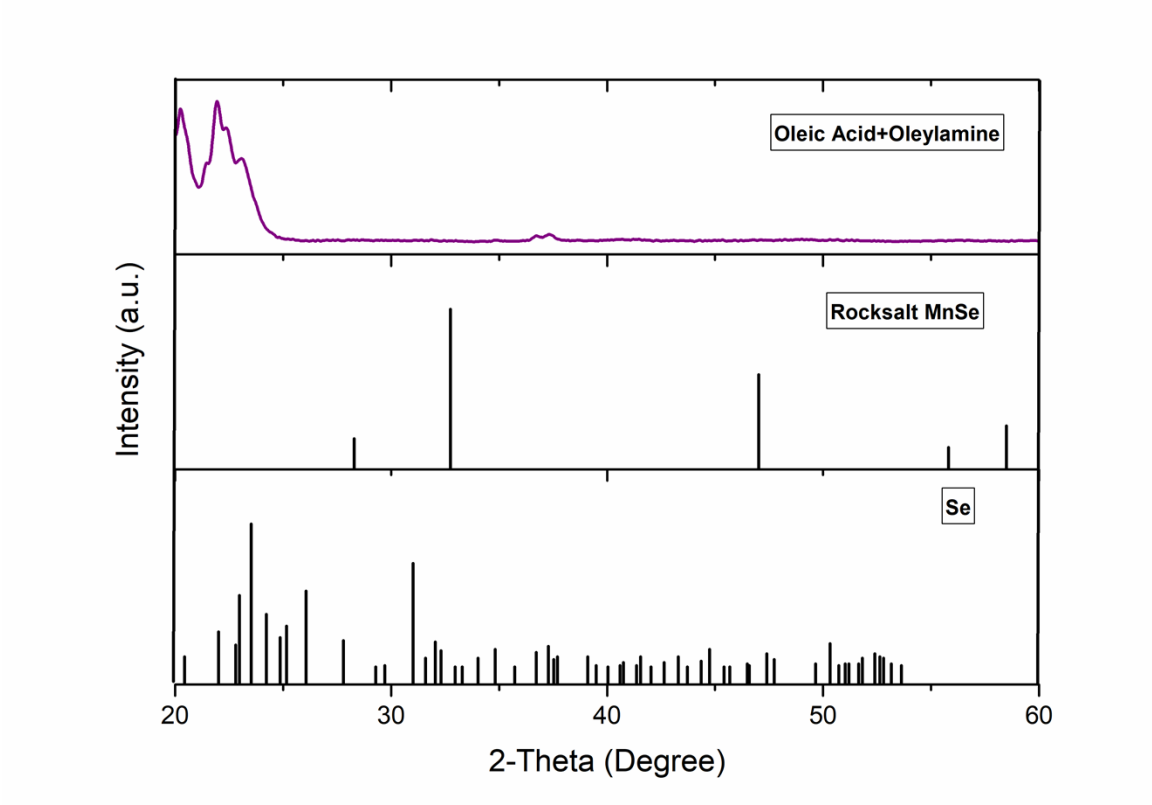


Figure S5. XRD pattern of sample synthesized with the oleic acid and oleylamine along with the Rocksalt.

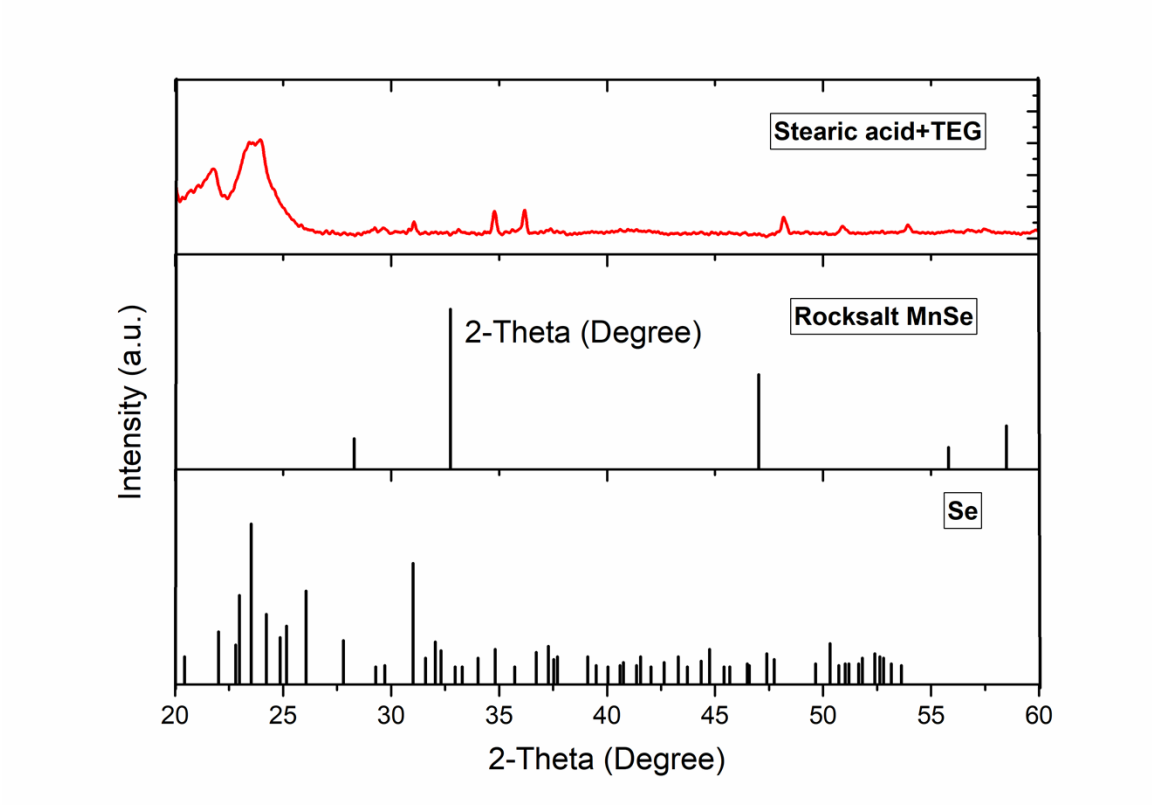


Figure S6. XRD pattern of sample synthesized with the stearic acid and octadecene along with the Rocksalt.

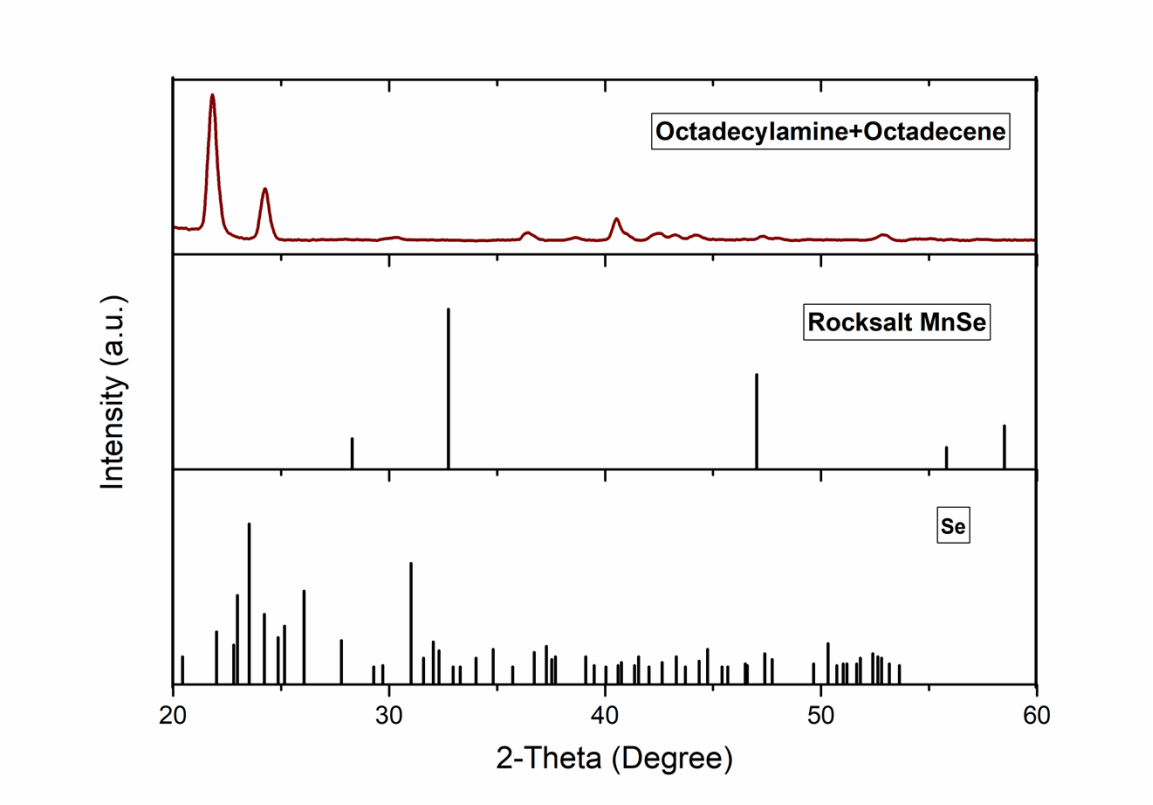


Figure S7. XRD pattern of sample synthesized with the combination of octadecylamine and octadecene along with the Rocksalt.

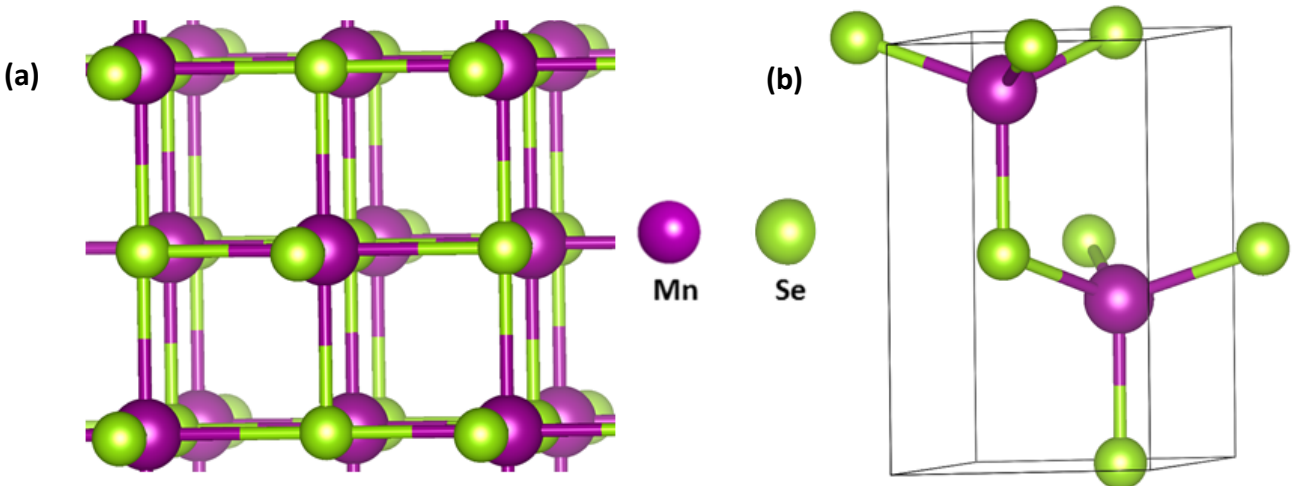


Figure S8. Crystal structure of a) Rocksalt/NS, b) Wurtzite/NNS of MnSe.

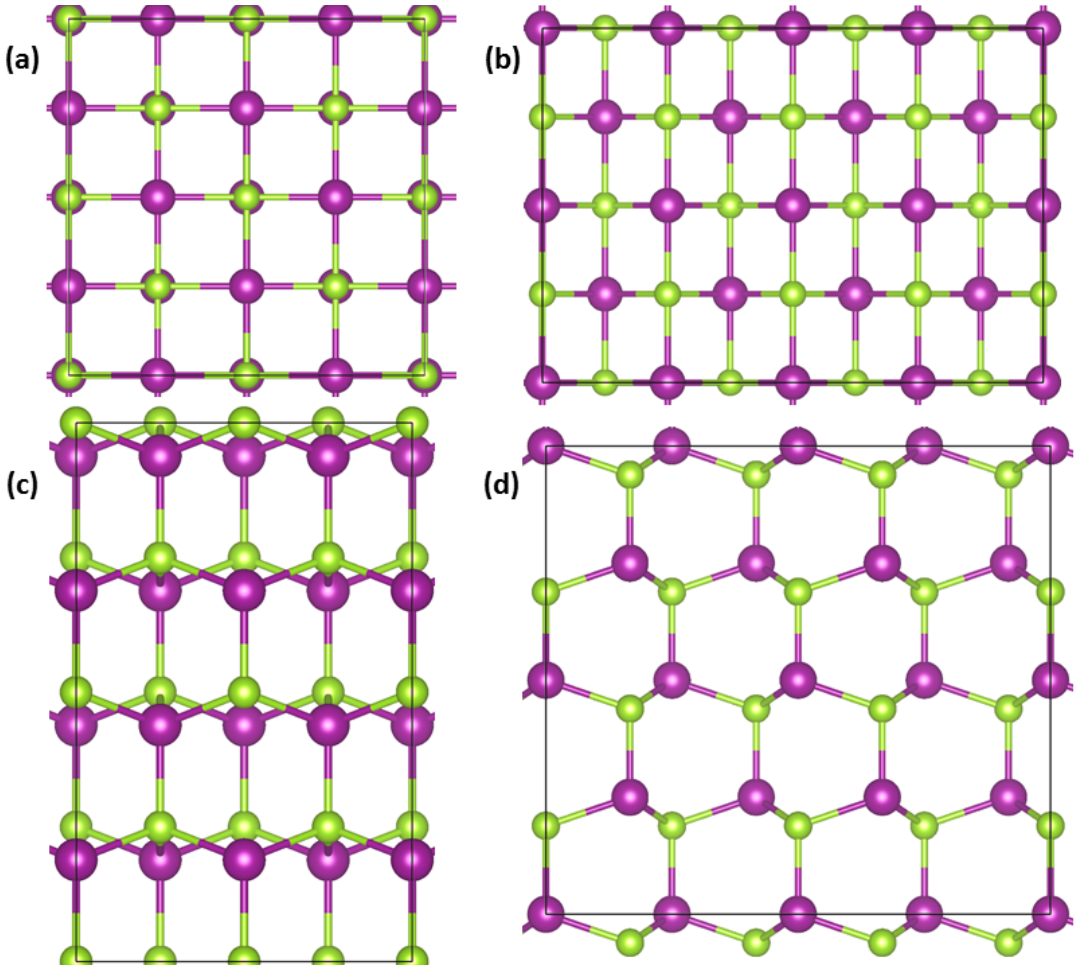


Figure S9. Top view of the crystal structures of (a) Rocksalt (100), (b) Rocksalt (110), (c) Wurtzite ($1\bar{0}10$) and (d) Wurtzite ($11\bar{2}0$) surfaces.

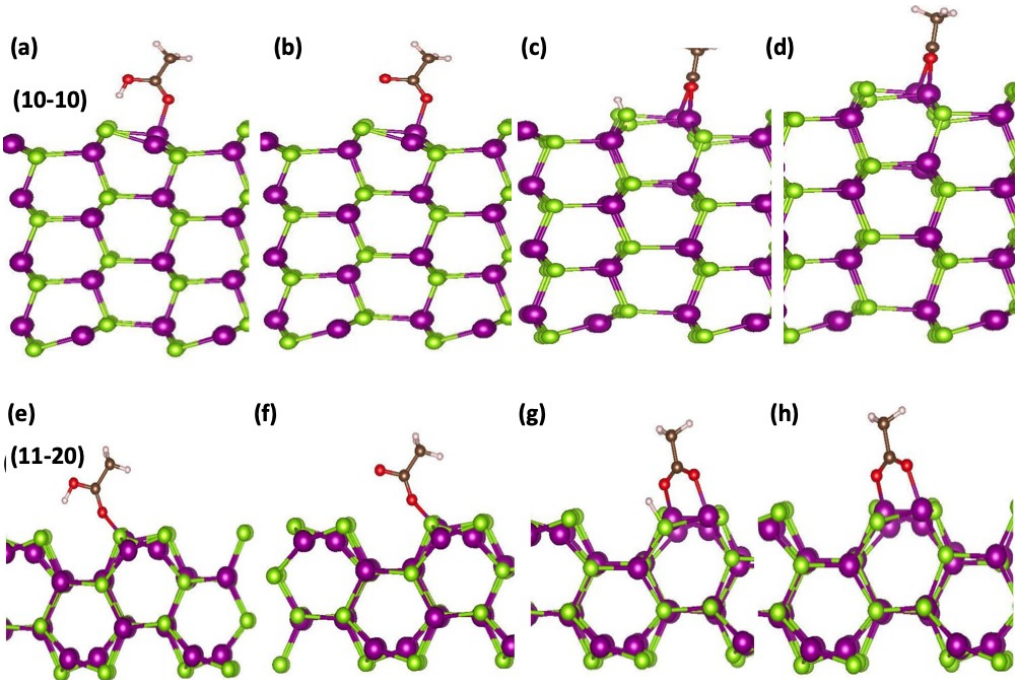


Figure S10. From left to right: a & e) Acetic acid (monodentate), (b & f) Acetate ion (monodentate), c & g) Acetic acid (bidentate), and d & h) Acetate ion (bidentate), adsorption on $(10\bar{1}0)$ and $(11\bar{2}0)$ surface of Wurtzite/NNS polymorph of MnSe.

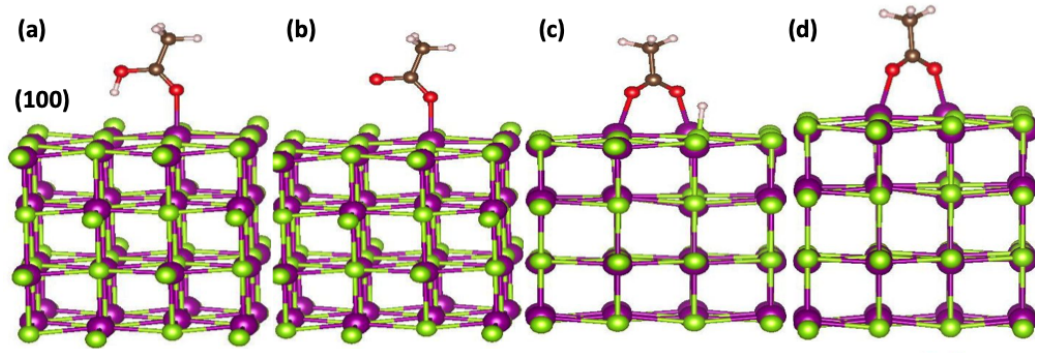


Figure S11. From left to right: a Acetic acid (monodentate), (b) Acetate ion (monodentate), c) Acetic acid (bidentate),, and d & h) Acetate ion (bidentate), adsorption on (100) surface of Rocksalt/NS polymorph of MnSe.

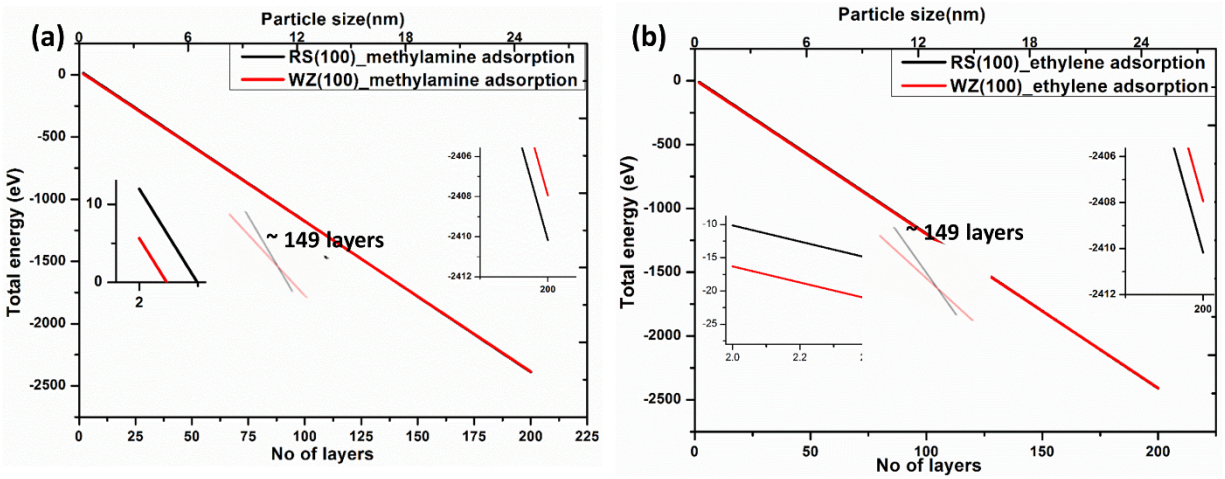


Figure S12. Total energy versus number of layers (particle size) plot of (a) methylamine (b) ethylene adsorption on (100) and $(10\bar{1}0)$ surfaces of Rocksalt/NS and Wurtzite/NNS polymorphs of MnSe.

Table S1. Surface energy of both the surfaces of Rocksalt and Wurtzite polymorphs of MnSe.

S.No.	**Different surfaces of MnSe polymorphs**	**Surface energy (j/m^2)**
1.	Rocksalt/NS (100 surface)	0.24 j /m^2
2.	Wurtzite/NNS $(10\bar{1}0)$ surface	0.23 j/m^2

3.	Wurtzite/NNS $(11\bar{2}0)$surface	0.27 j/m^2

Table S2. Bader charge of both the surfaces of Rocksalt and Wurtzite polymorphs of MnSe.

S.No.	**Polymorphs of MnSe**	**On bare Mn atom**	**Acetate adsorption**	**Methylamine adsorption**	**Ethylene group adsorption**

1.	Rocksalt/NS (110 surface)	1.13	1.21	1.17	1.12
2.	Wurtzite/NNS $(10\bar{1}0)/(100)$ surface	1.12	1.22	1.15	1.10