Supplementary Information for

"Interaction of III-As Monolayer with SARS-CoV-2 Biomarkers: Implications for Biosensor Development"

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A. Charge Density Difference

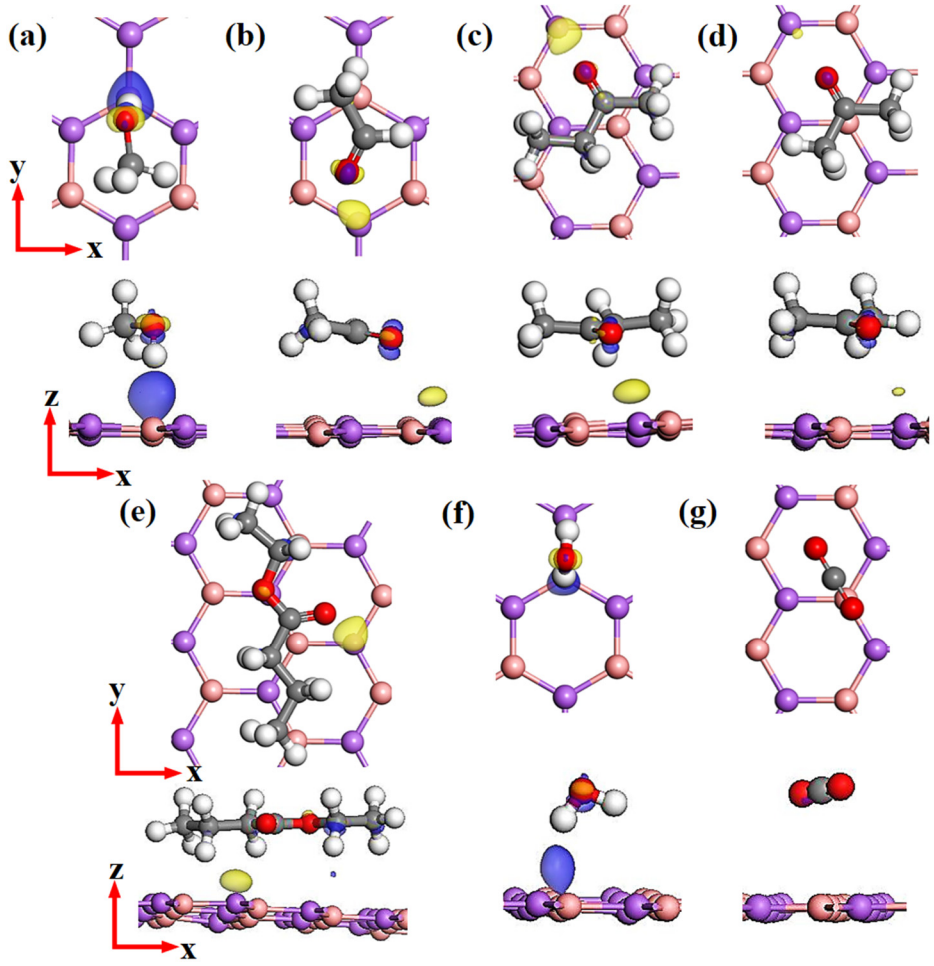

Figure S1. Charge density difference of the most optimized structure (top and side view) for (a) Methanol, (b) Ethanal, (c) Butanone, (d)Acetone, (e) Ethyl Butyrate, (f) H_2O and (g) CO_2 on pristine BAs monolayer. Blue region indicates charge accumulation, and yellow region indicates charge depletion.

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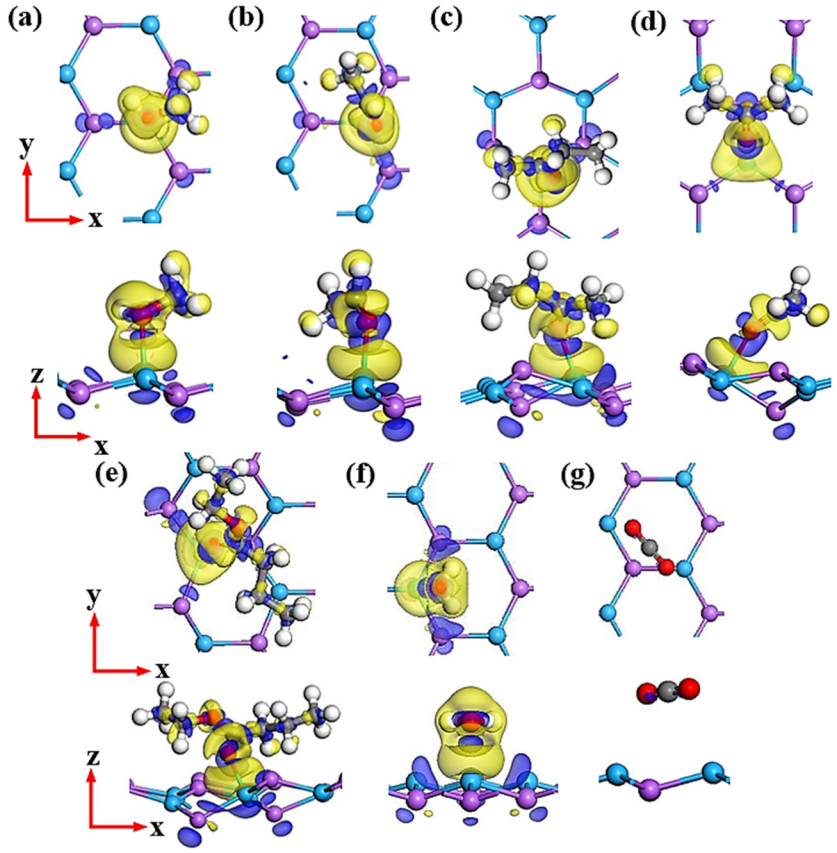

Figure S2. Charge density difference of the most optimized structure (top and side view) for (a) Methanol, (b) Ethanal, (c) Butanone, (d) Acetone, (e) Ethyl Butyrate, (f) H_2O and (g) CO_2 on pristine GaAs monolayer. Blue region indicates charge accumulation, and yellow region indicates charge depletion.

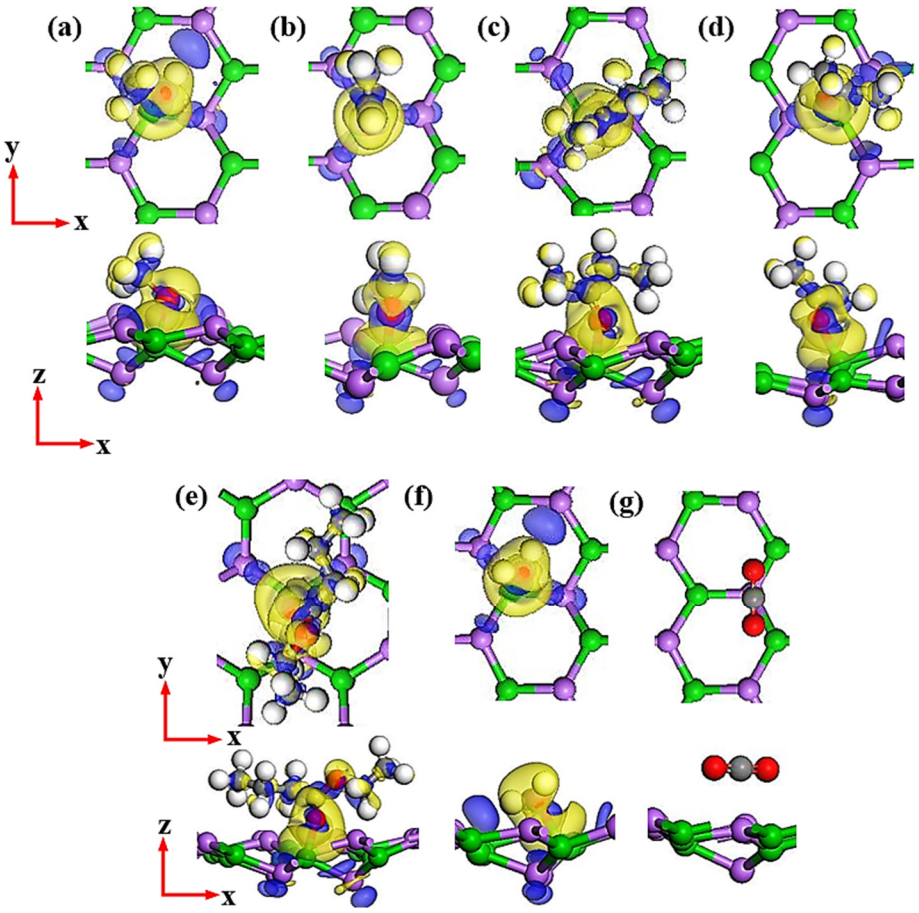

Figure S3. Charge density difference of the most optimized structure (top and side view) for (a) Methanol, (b) Ethanal, (c) Butanone, (d) Acetone, (e) Ethyl Butyrate, (f) H_2O and (g) CO_2 on pristine AlAs monolayer. Blue region indicates charge accumulation, and yellow region indicates charge depletion.

B. Partial Density of states (PDOS) for III-As Analyte system.

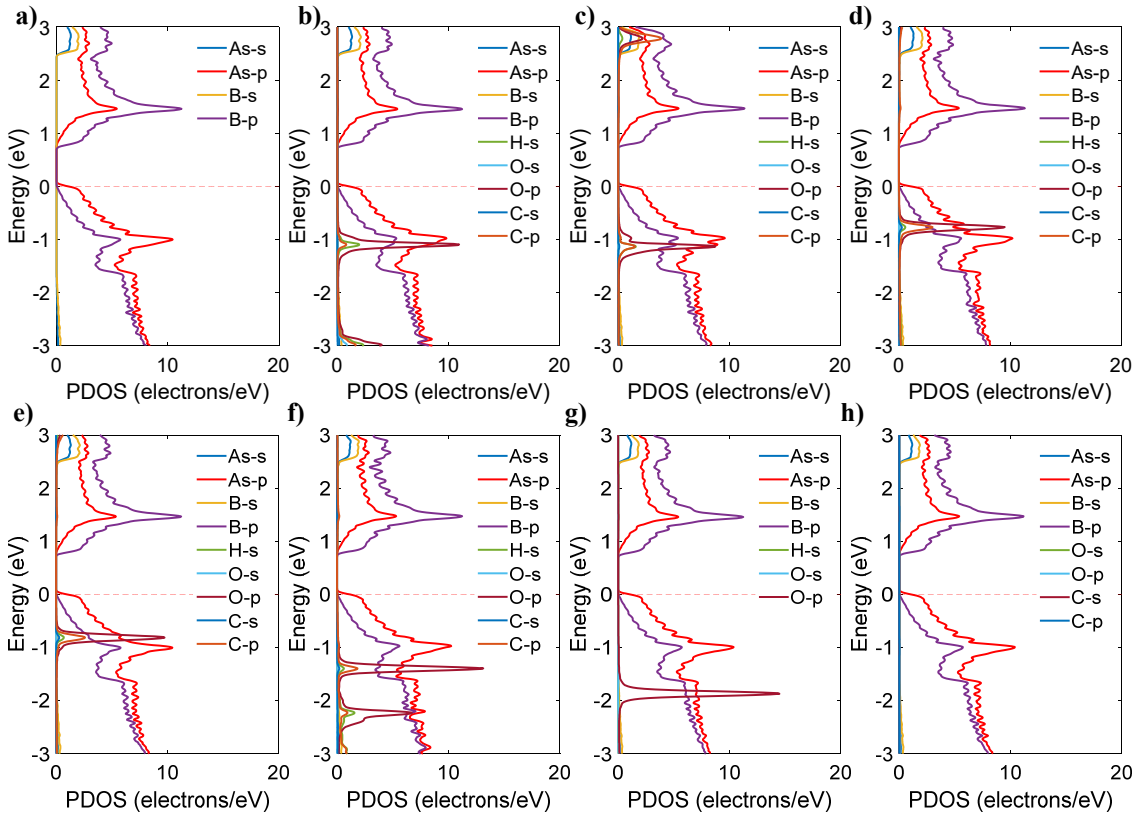

Figure S4. PDOS of (a) pristine BAs (b) Methanol (c) Ethanal (d) Butanone (e) Acetone (f) Ethyl Butyrate (g) H_2O and (h)CO_2 adsorbed structure on BAs.

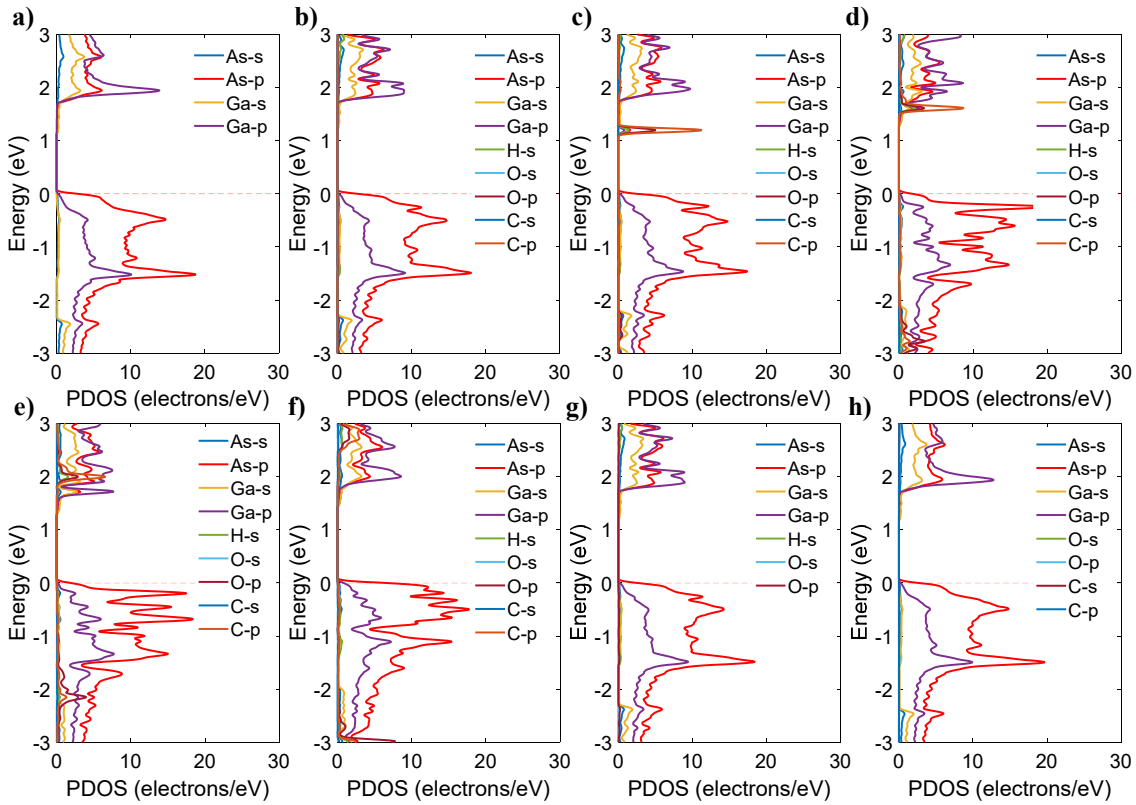

Figure S5. PDOS of (a) pristine GaAs (b) Methanol (c) Ethanal (d) Butanone (e) Acetone (f) Ethyl Butyrate (g) H_2O and (h)CO_2 adsorbed structure on GaAs.

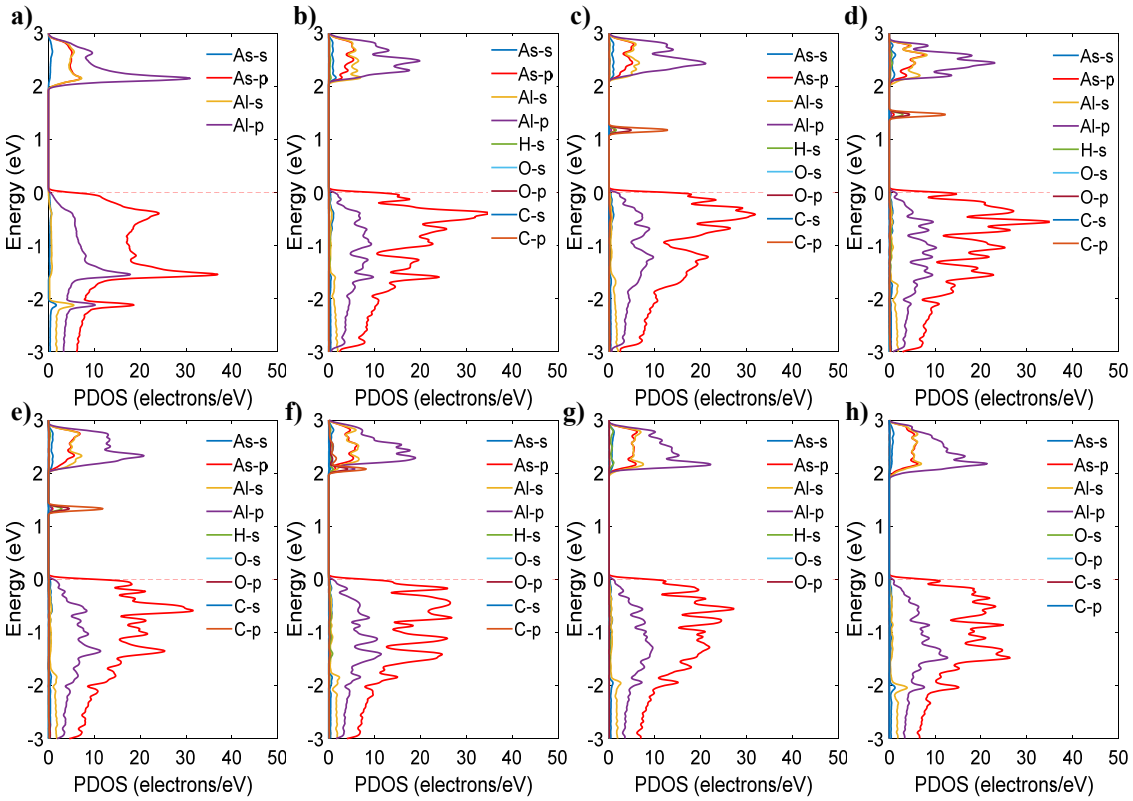

Figure S6. PDOS of (a) pristine AlAs (b) Methanol (c) Ethanal (d)Butanone (e) Acetone (f) Ethyl Butyrate (g) H_2O and (h)CO_2 adsorbed structure on AlAs.

C. Loss Factor:

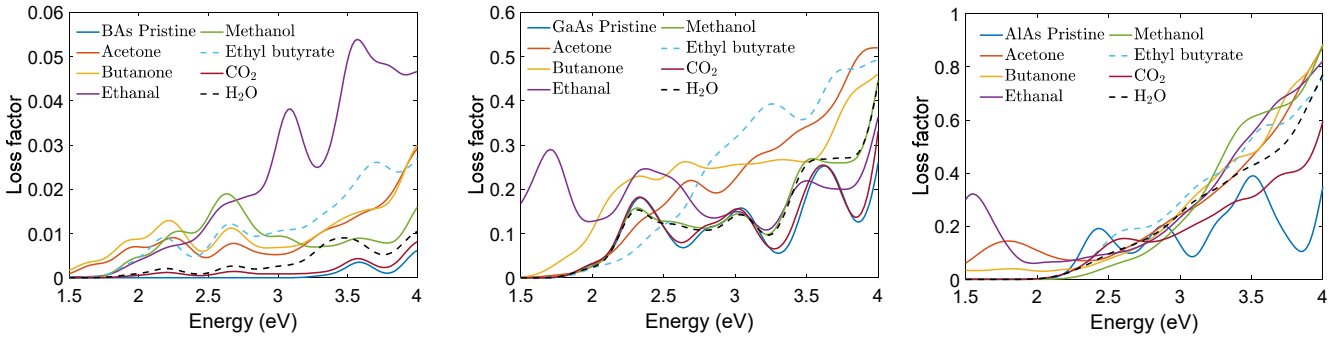

Figure S7. Loss factor vs energy for BAs, GaAs & AlAs analyte system

D. Phonon Dispersion:

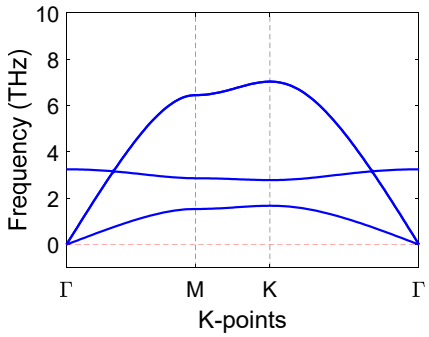

Figure S8. Phonon dispersion of AlAs unit cell

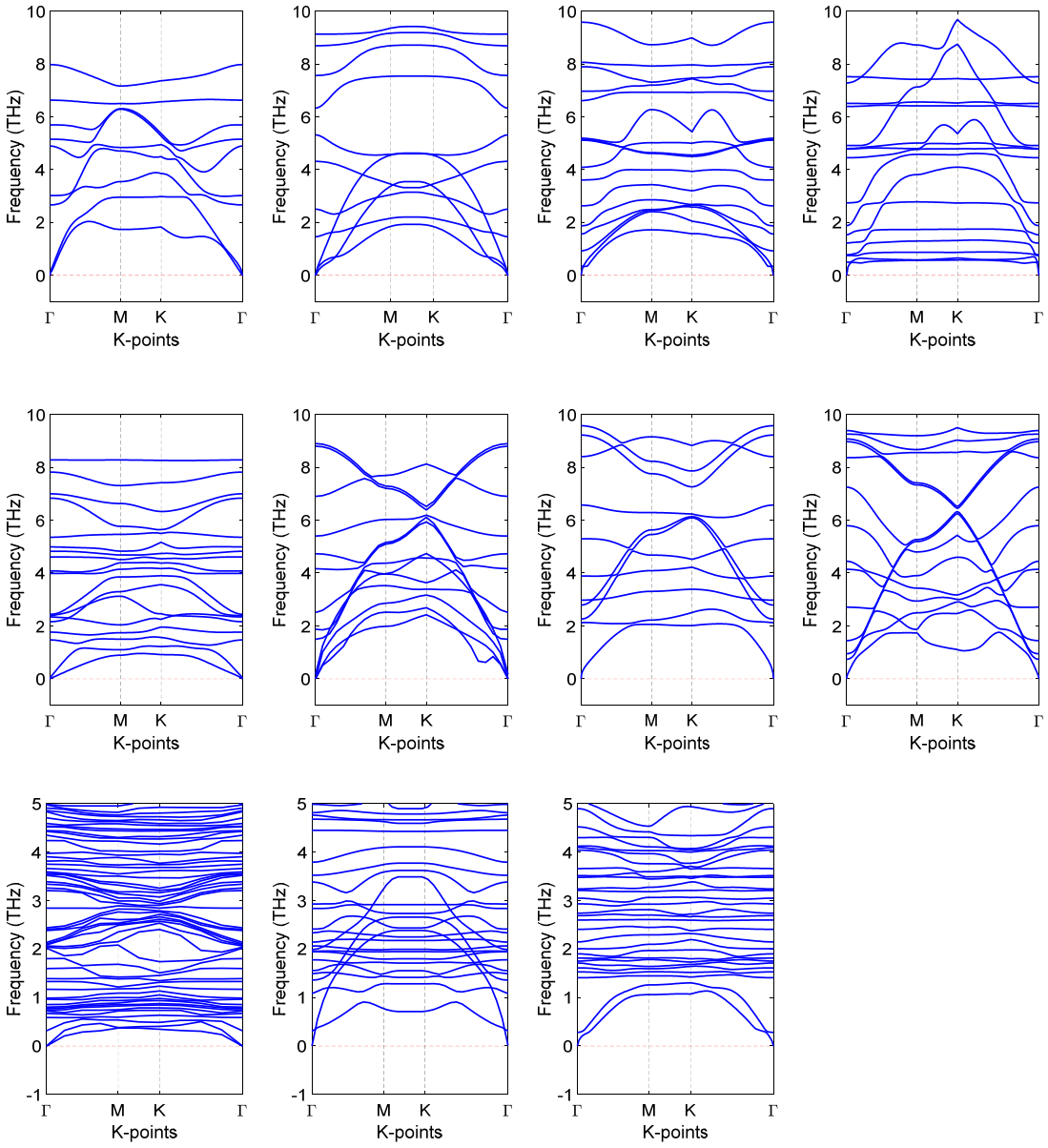

Figure S9. Phonon dispersion of (a) methanol on AlAs unit cell, (b) acetone on AlAs unit cell, (c) butanone on AlAs unit cell, (d) ethyl butyrate on AlAs unit cell, (e) H_2O on AlAs unit cell ,(f) ethanal on GaAs unit cell, (g) acetone on GaAs unit cell (h) butanone on GaAs unit cell , (i) ethanal on AlAs 4×4 cell , (j) methanol on GaAs 4×4 cell and (k) ethyl butyrate on GaAs 4×4 cell