

Supplementary file

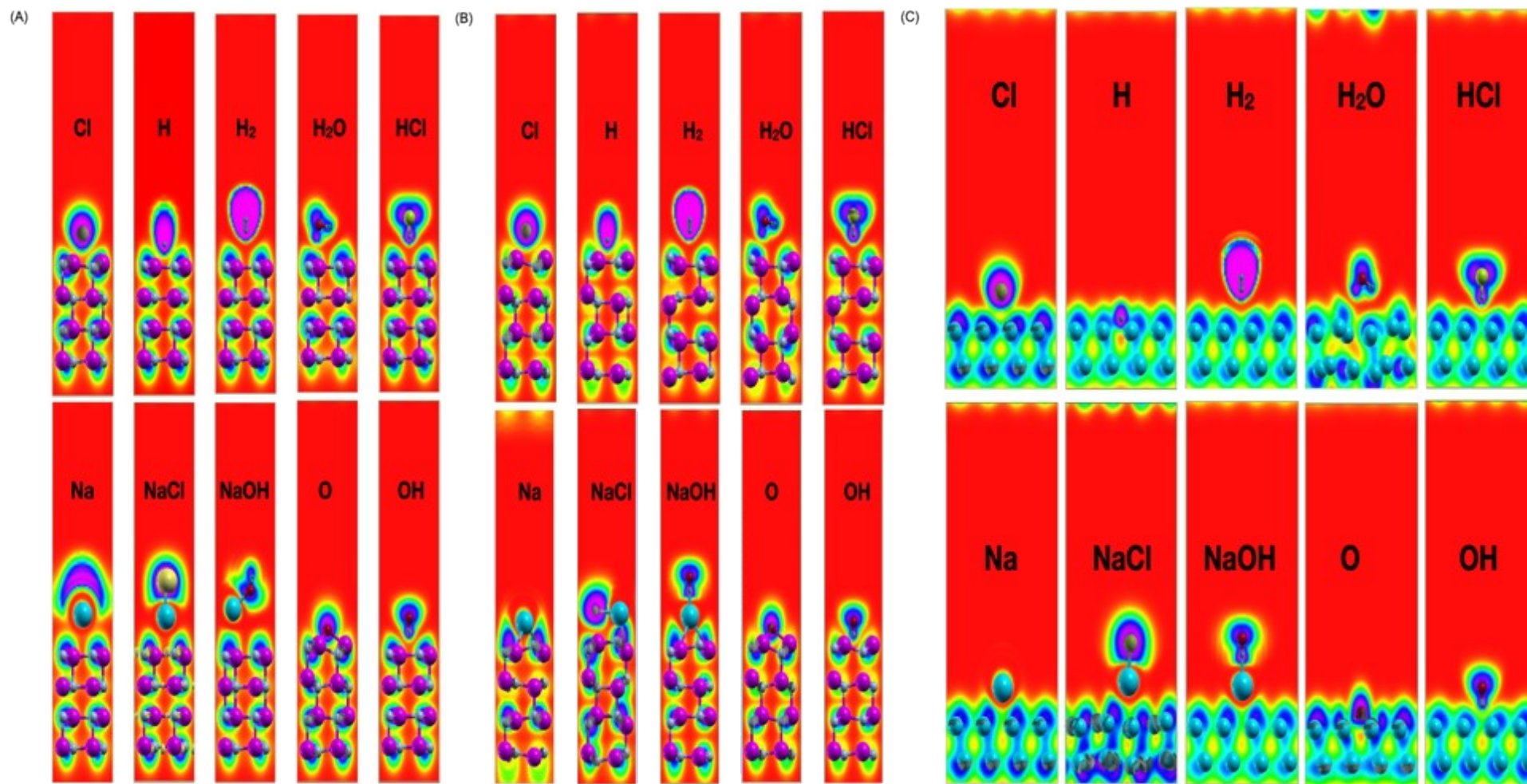
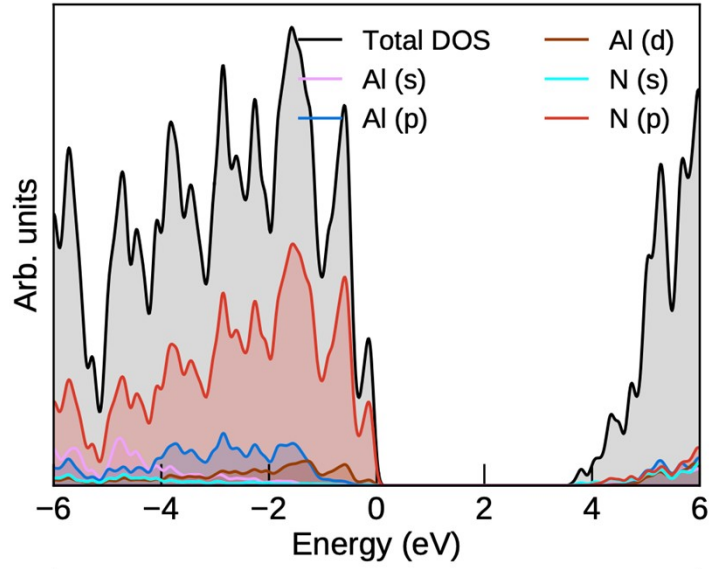
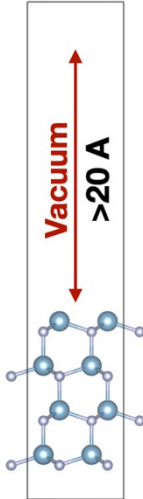
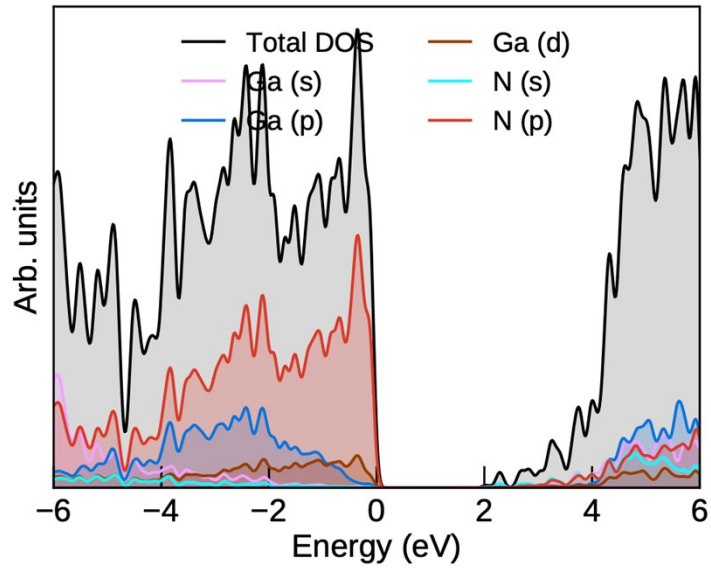
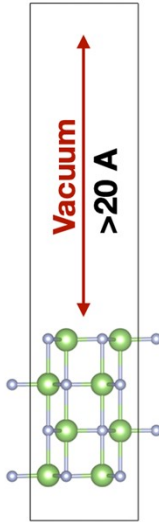


Figure S1: Electron localization function of the complex systems comprising of the molecules and ions adsorbed on different surfaces with VdW forces (A) on AlN surface (B) GaN surface (C) Si surface.

AlN (001) surface



GaN (001) surface



Si (001) surface

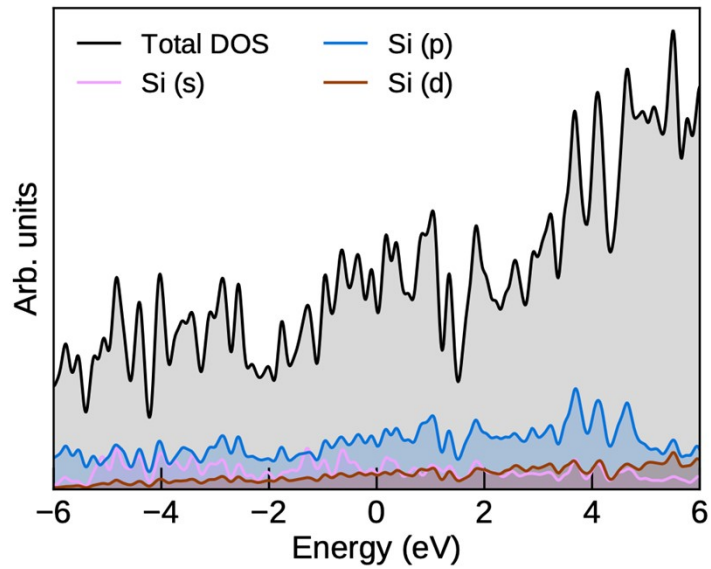
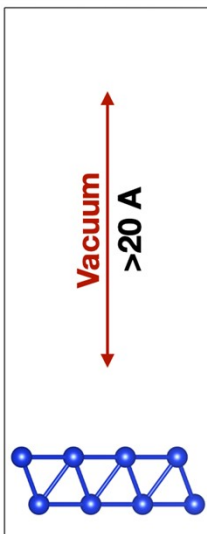


Figure S2: Projected Density of States of the pristine surfaces with VdW forces.

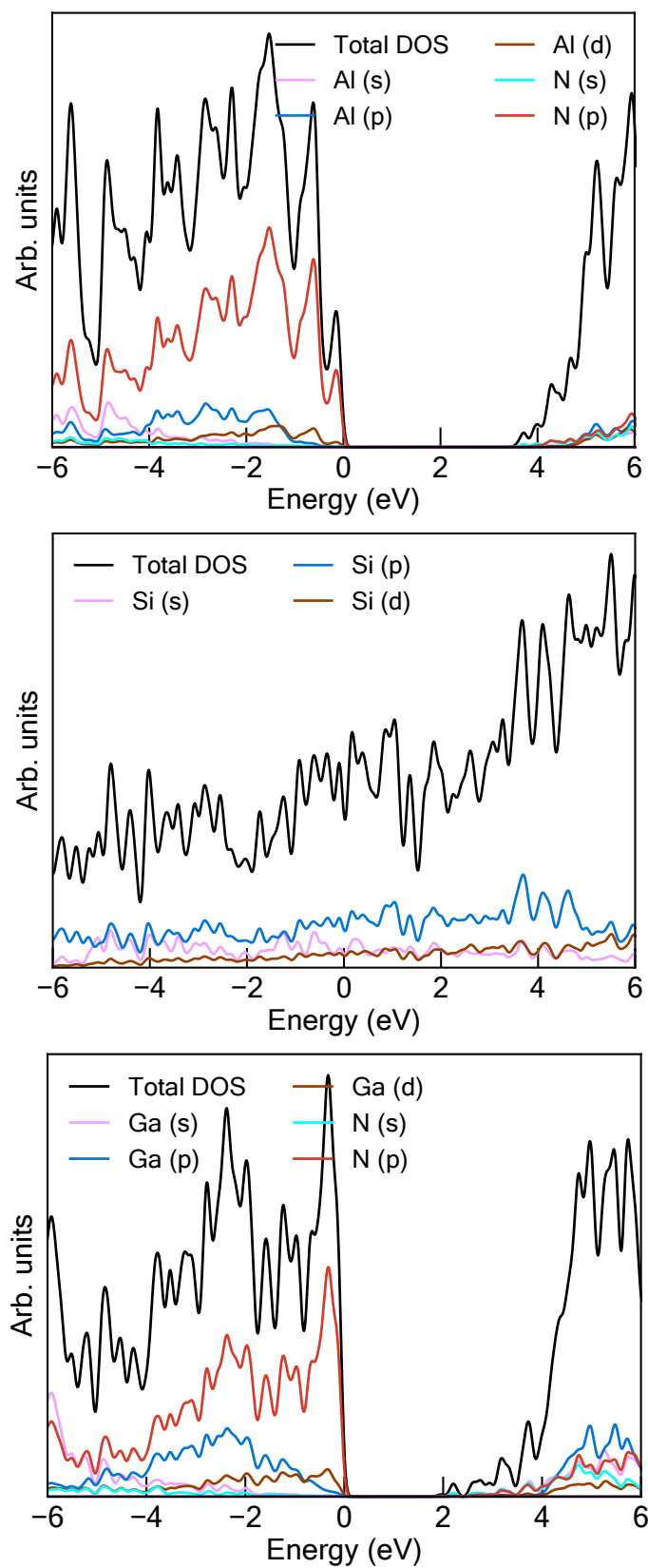


Figure S3: Projected Density of States of the pristine surfaces without VdW forces.