Supplementary Materials for Aluminene nanoribbons: Work function tuning with strain and surface termination

Sampriti Shome and Nirat Ray*

Department of Materials Science and Engineering, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India

E-mail: nirat@iitd.ac.in

Supplementary Information

The Supplementary Information provides additional electronic and electrostatic details supporting the main text. It includes the calculated electronic band structures of H-, OH-, and F-passivated zigzag aluminene nanoribbons under various uniaxial strain conditions. In addition, the planar-averaged and macroscopic-averaged electrostatic potential profiles are presented for all considered models, namely H-, O-, F-, and OH-passivated zigzag and armchair nanoribbons, evaluated under compressive and tensile strains of -5%, -2.5%, 0%, $+2.5\%$, and $+5\%$. For completeness and comparison, the electrostatic potential profiles of pristine zigzag and armchair aluminene nanoribbons, as well as the pristine two-dimensional aluminene sheet, are also included. These results provide the reference vacuum levels used for work-function estimation and offer further insight into the strain- and edge-dependent charge redistribution mechanisms discussed in the main manuscript.

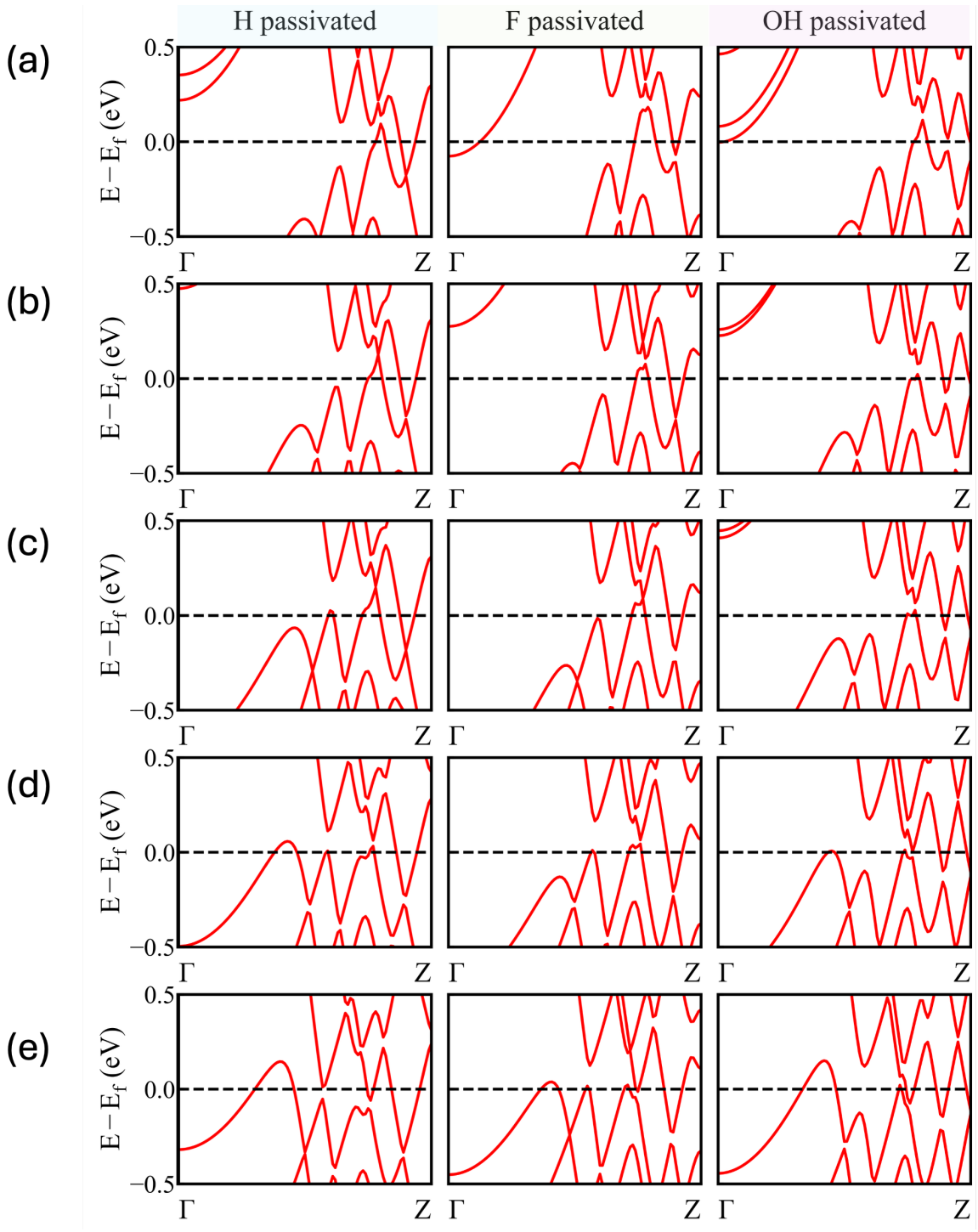

Figure S1: Bandstructure plot of zigzag passivated nanoribbon under (a)-5% (b)-2.5% (c)0% (d)+2.5% (e)+5% strain

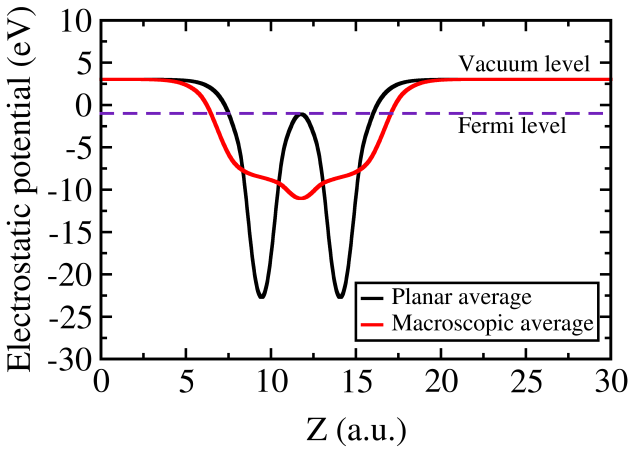

Figure S2: Work function plot of 2D aluminene sheet.

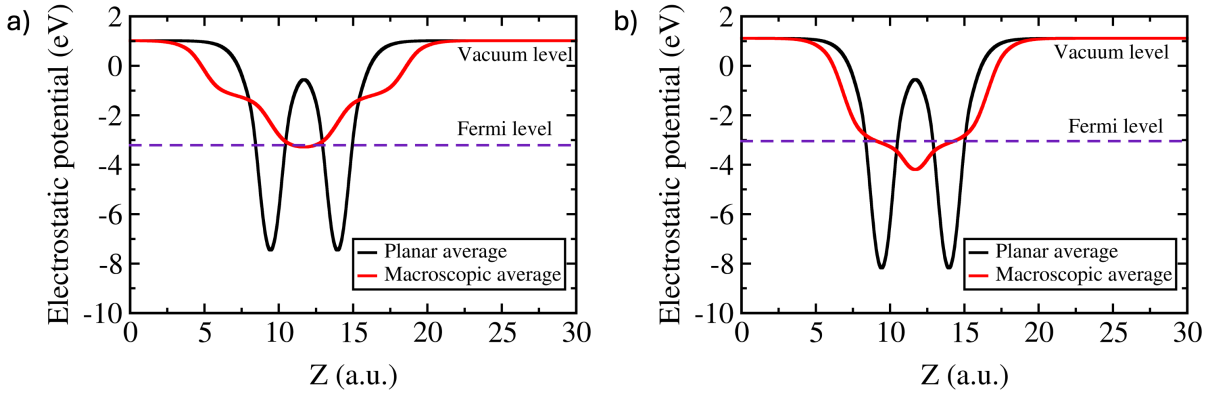

Figure S3: Work function plot of pristine aluminene nanoribbons (a) 3p armchair configuration (b) zigzag configuration.

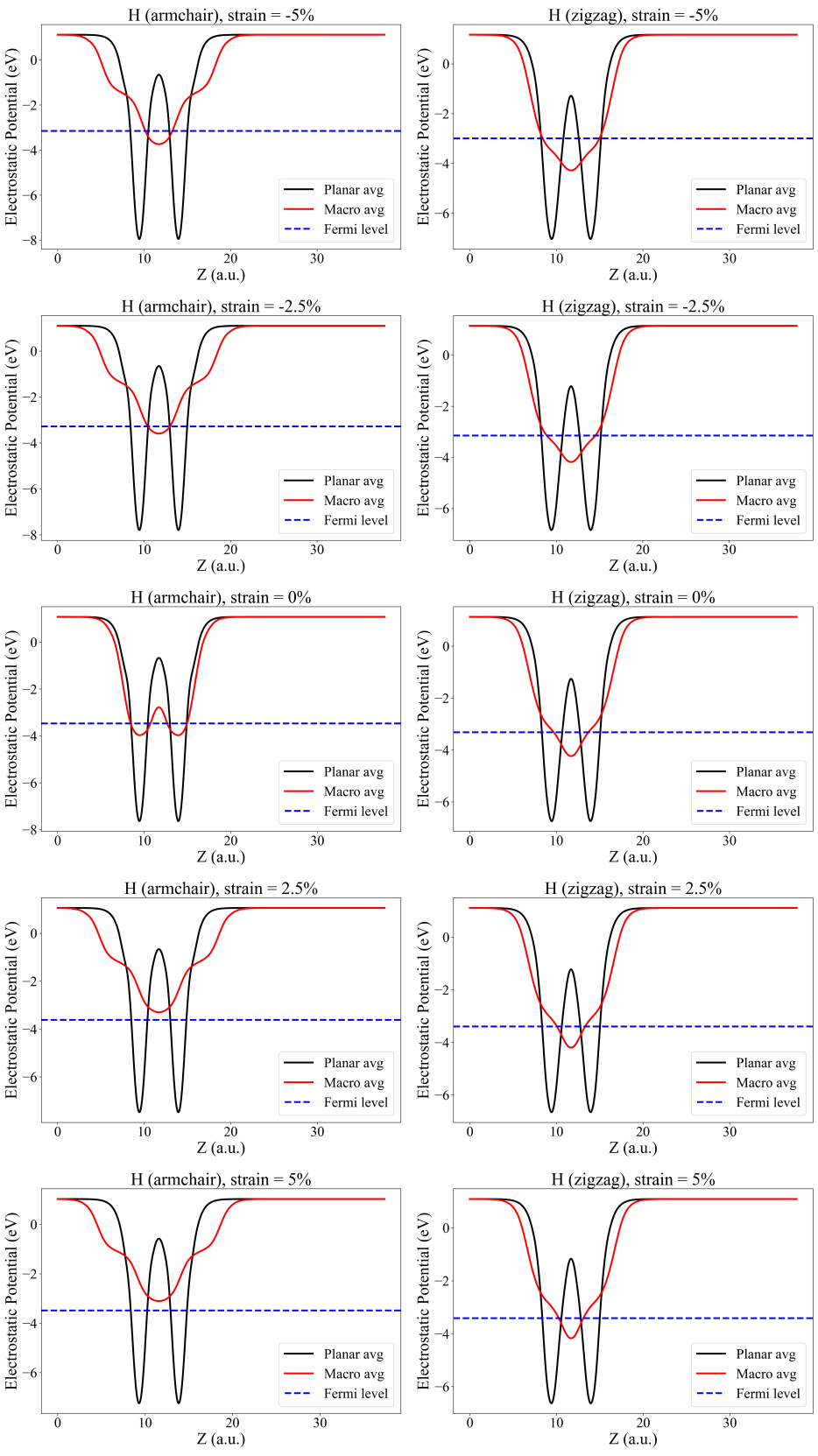

Figure S4: Electrostatic potential plot of H-atom passivated aluminene nanoribbons

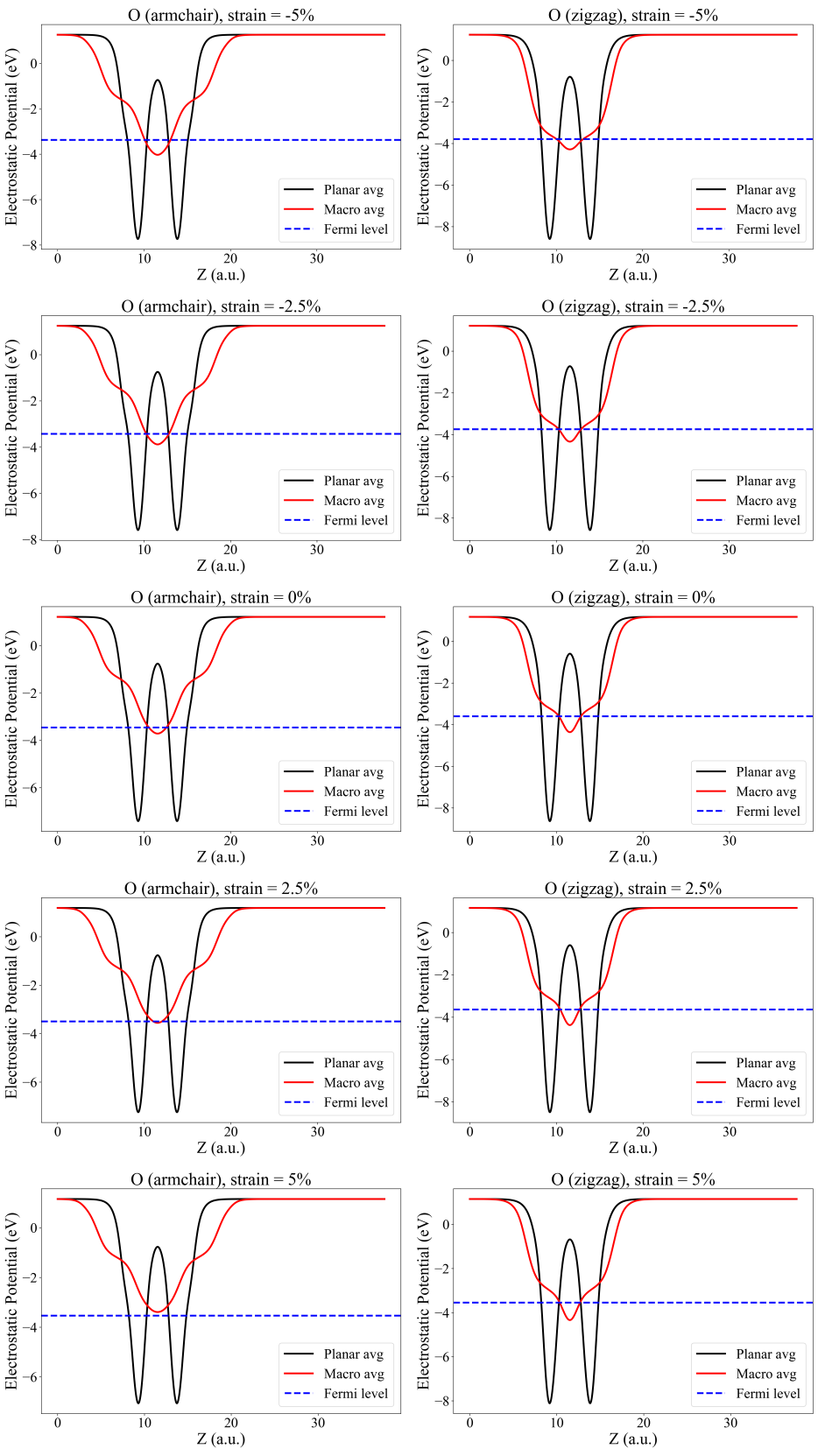

Figure S5: Electrostatic potential plot of O-atom passivated aluminene nanoribbons

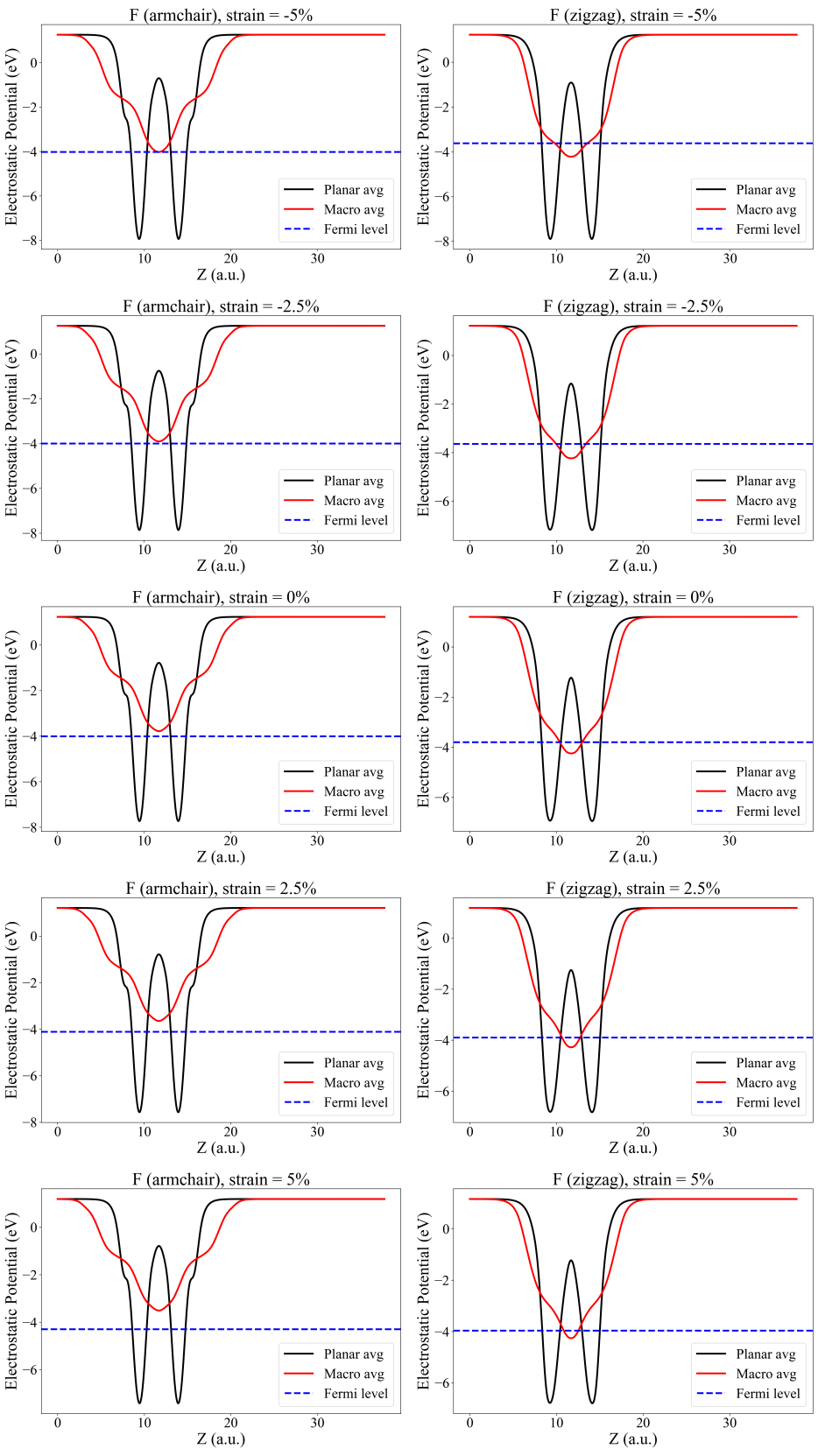

Figure S6: Electrostatic potential plot of F-atom passivated aluminene nanoribbons

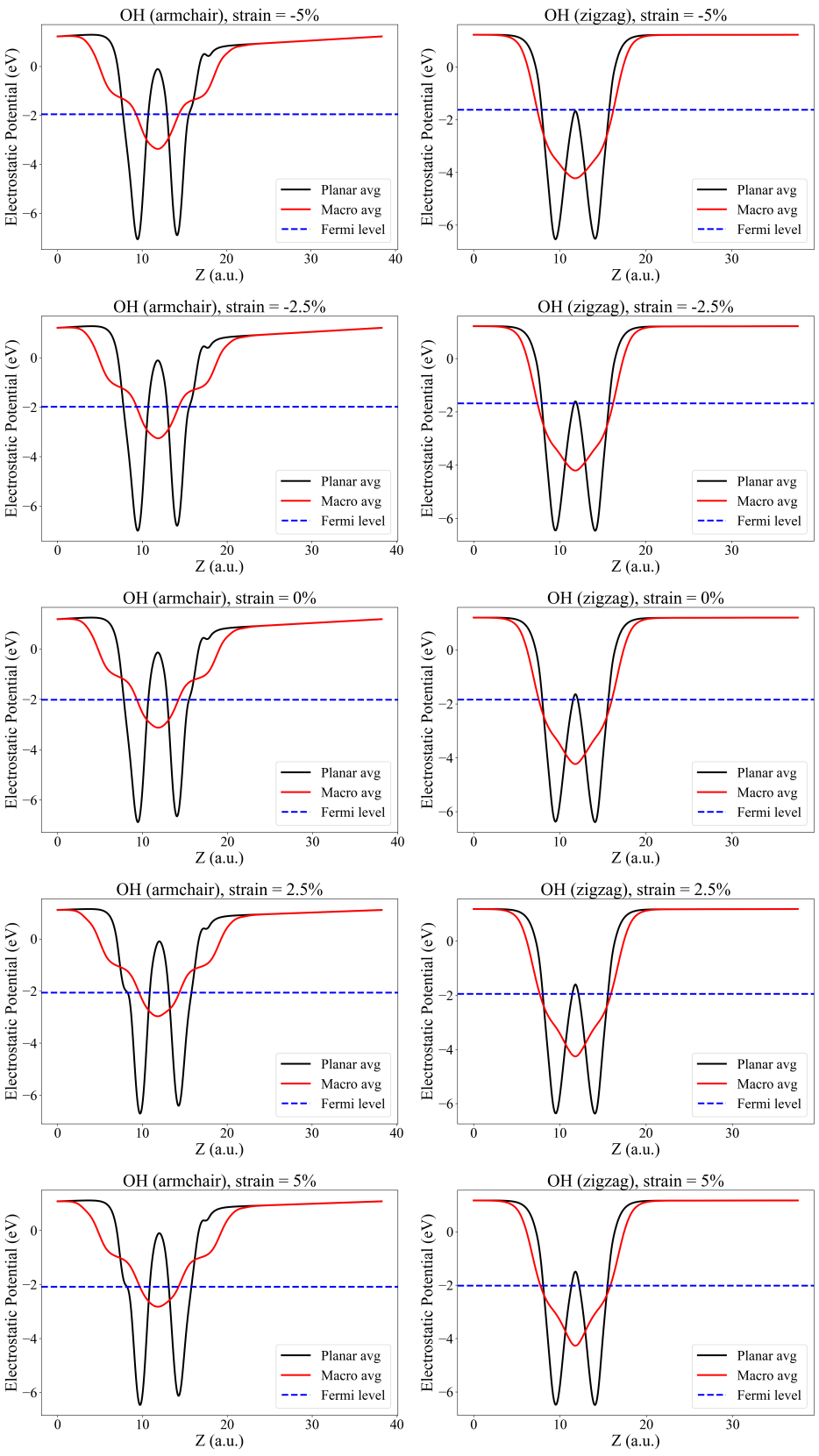

Figure S7: Electrostatic potential plot of OH-atom passivated aluminene nanoribbons

Table 1: Edge formation energy per unit length of passivated aluminene nanoribbons.

Passivation	**Formation energy (eV/Å)**	
	Armchair	**Zigzag**
H	-0.84	-0.98
O	-2.56	-2.63
F	-2.63	-2.45
OH	-2.44	-2.60

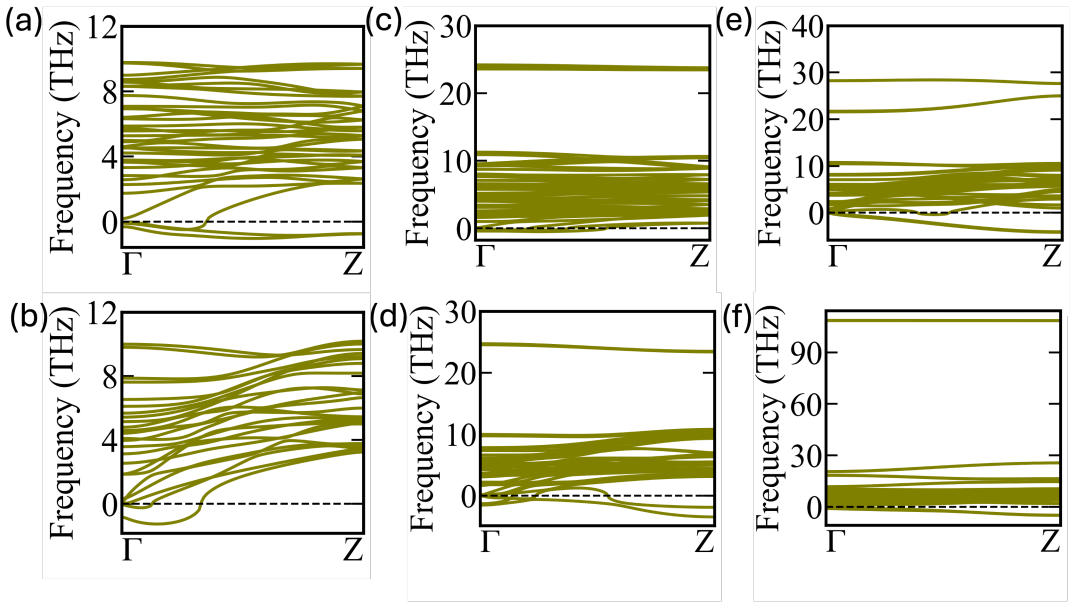

Figure S8: Phonon dispersion spectra for (a) Pristine armchair, (b) Pristine zigzag, (c) F passivated armchair, (d) F passivated zigzag, (e) O passivated zigzag (f) OH passivated zigzag