

Defect-enriched tunability of electronic and charge-carrier transport characteristics of 2D Borocarbonitride (BCN) monolayers from ab initio calculations

Vivek K. Yadav^a, Himanshu Chakraborty^a, Michael L. Klein^{a,*}, Umesh V. Waghmare^b, C.N.R. Rao^c

a. Department of Chemistry and Institute for Computational Molecular Science (ICMS), Temple University, Philadelphia, USA 19122

b. Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, P.O Jakkur, Bangalore 560064, India

c. International Center for Materials Science, Jawaharlal Nehru Centre for Advanced Scientific Research, P.O Jakkur, Bangalore 560064, India

Supporting Information

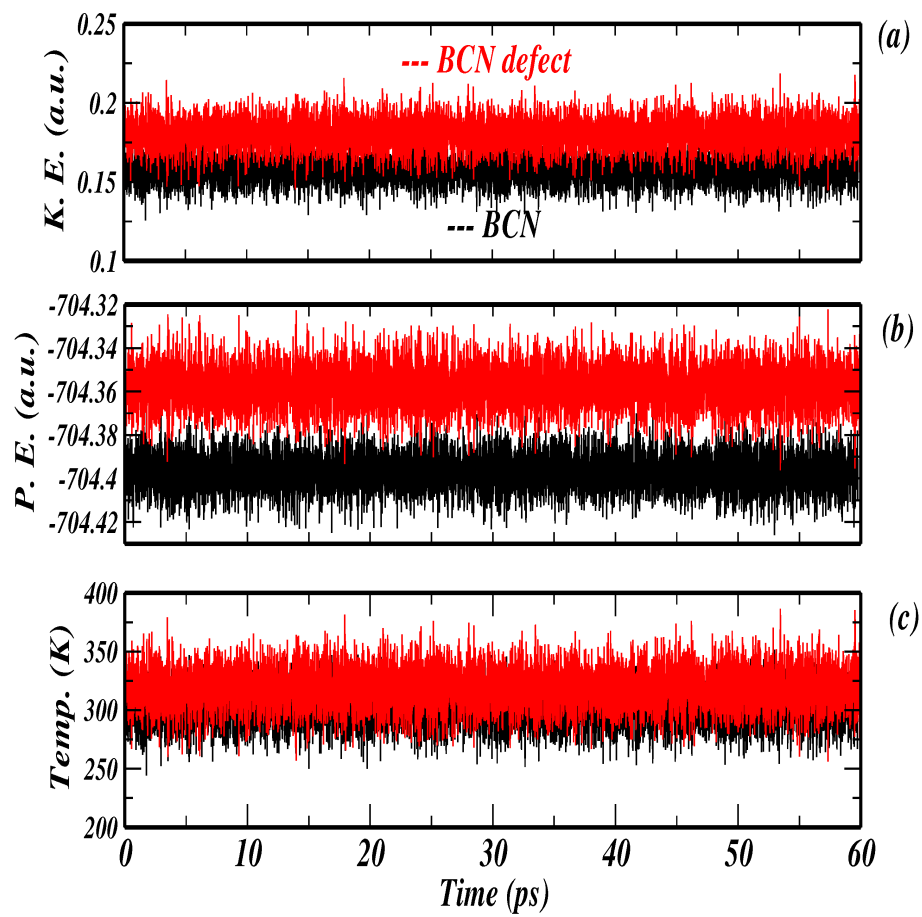


Fig. 1 SI-1: Time evolution of the (a) Kinetic Energy, (b) Potential Energy, and (c) Temperature (K) of the BCN and BCN-defect configuration (Fig 1), respectively. The energy is expressed in Atomic Units (a.u.)

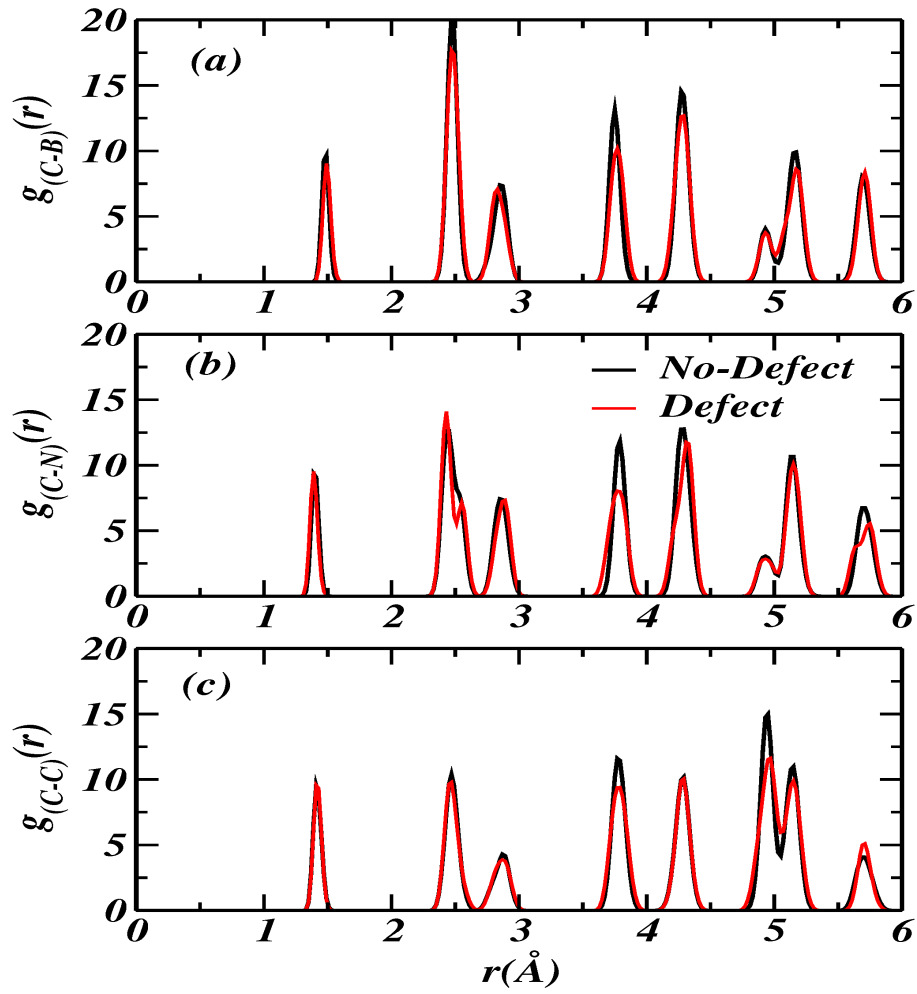


Fig. 2 SI-2: RDF of Carbon with (a) Boron, (b) Nitrogen, and (c) Carbon for BCN and BCN-defect configuration (Fig 1).

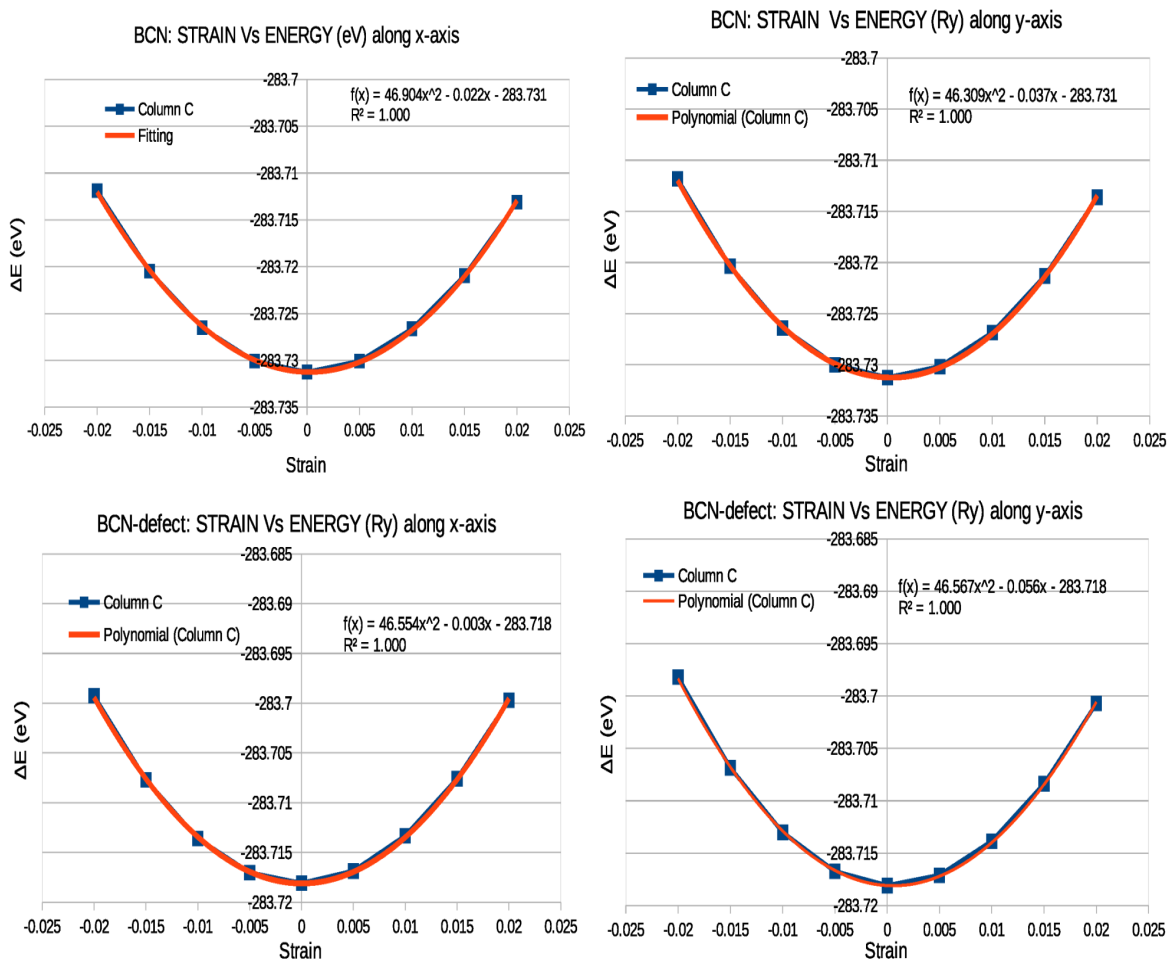


Fig. 3 SI-3a: Energy-strain relationship for BCN and BCN-defect configuration (Fig 1).

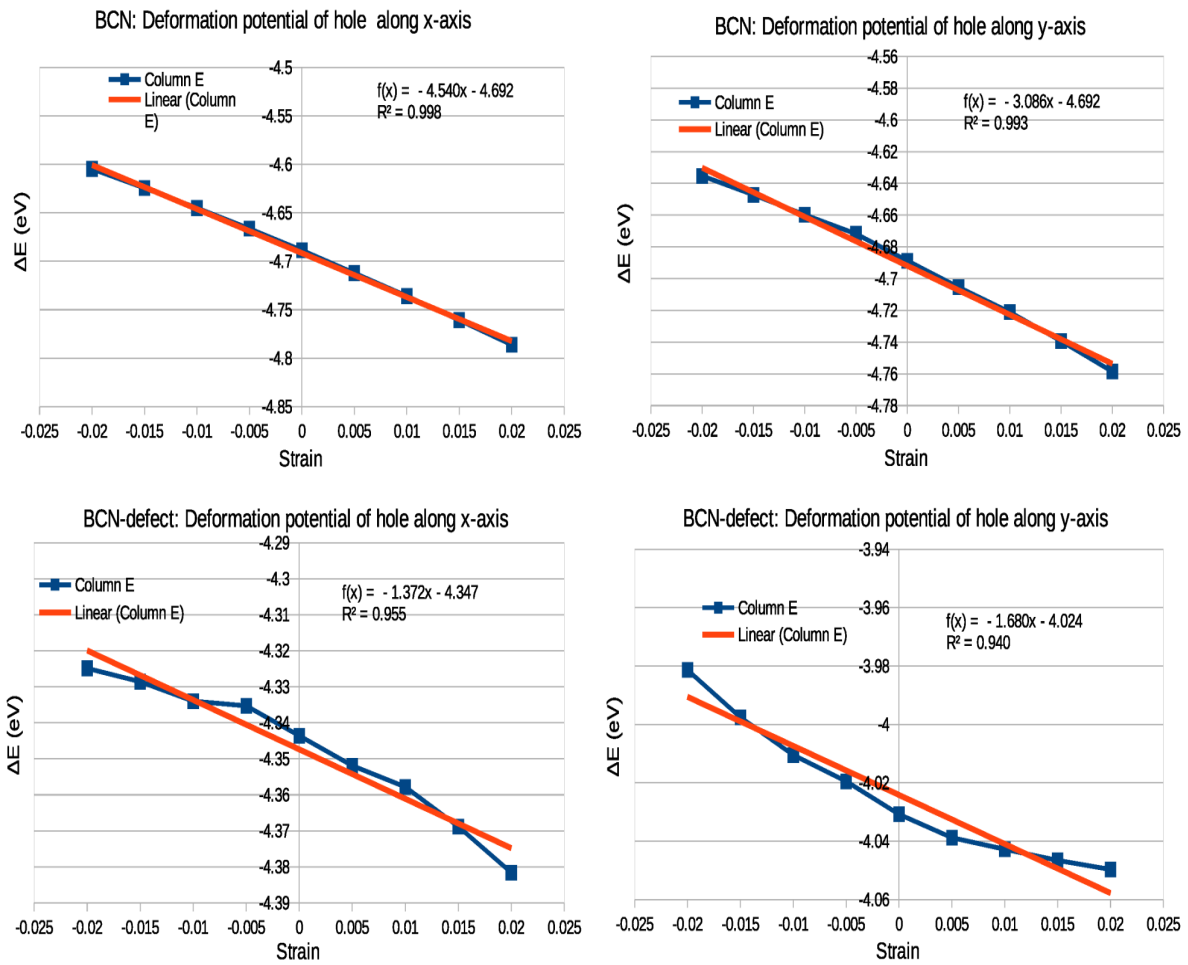


Fig. 4 SI-3b: Shifts of valence band under uniaxial strain for BCN and BCN-defect configuration (Fig 1).

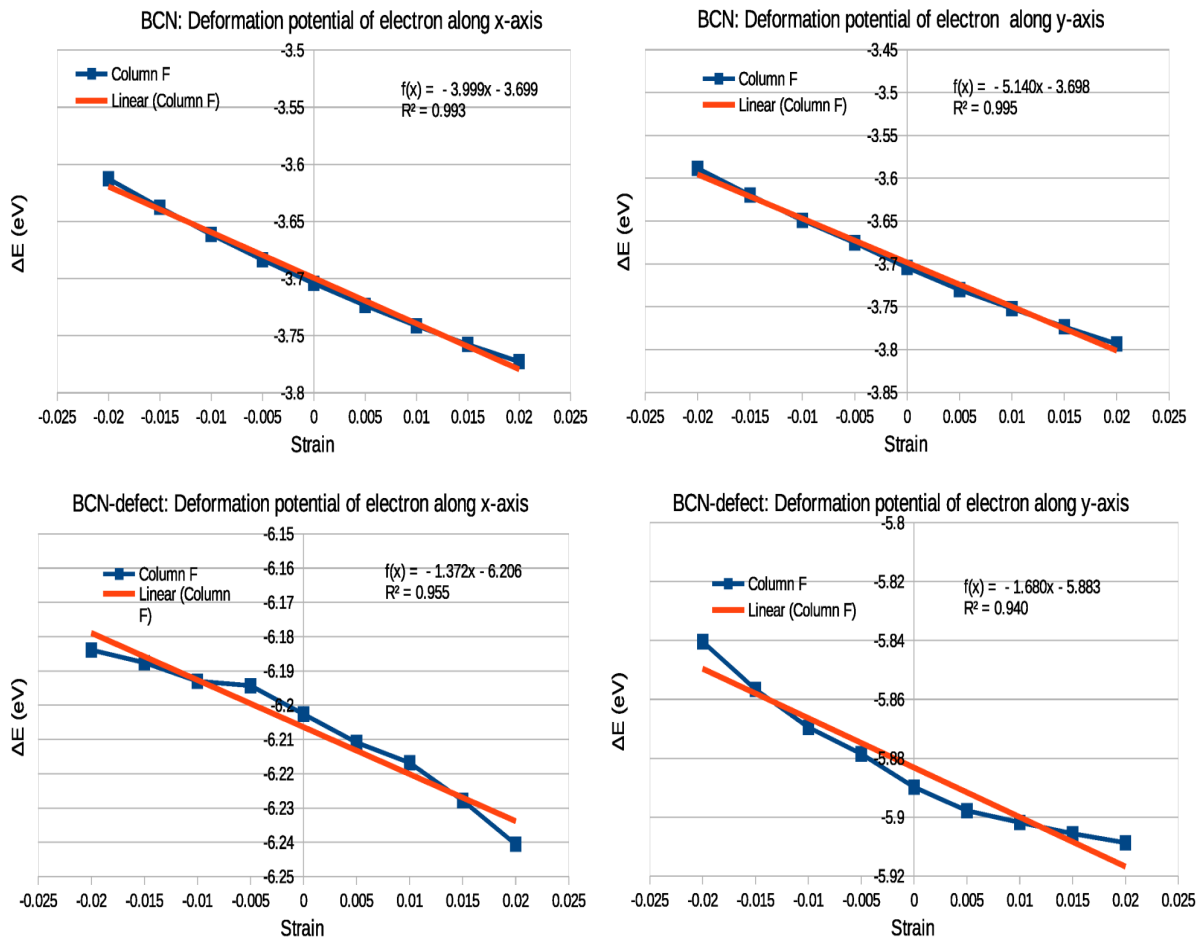


Fig. 5 SI-3c: Shifts of conduction band under uniaxial strain for BCN and BCN-defect configuration (Fig 1).

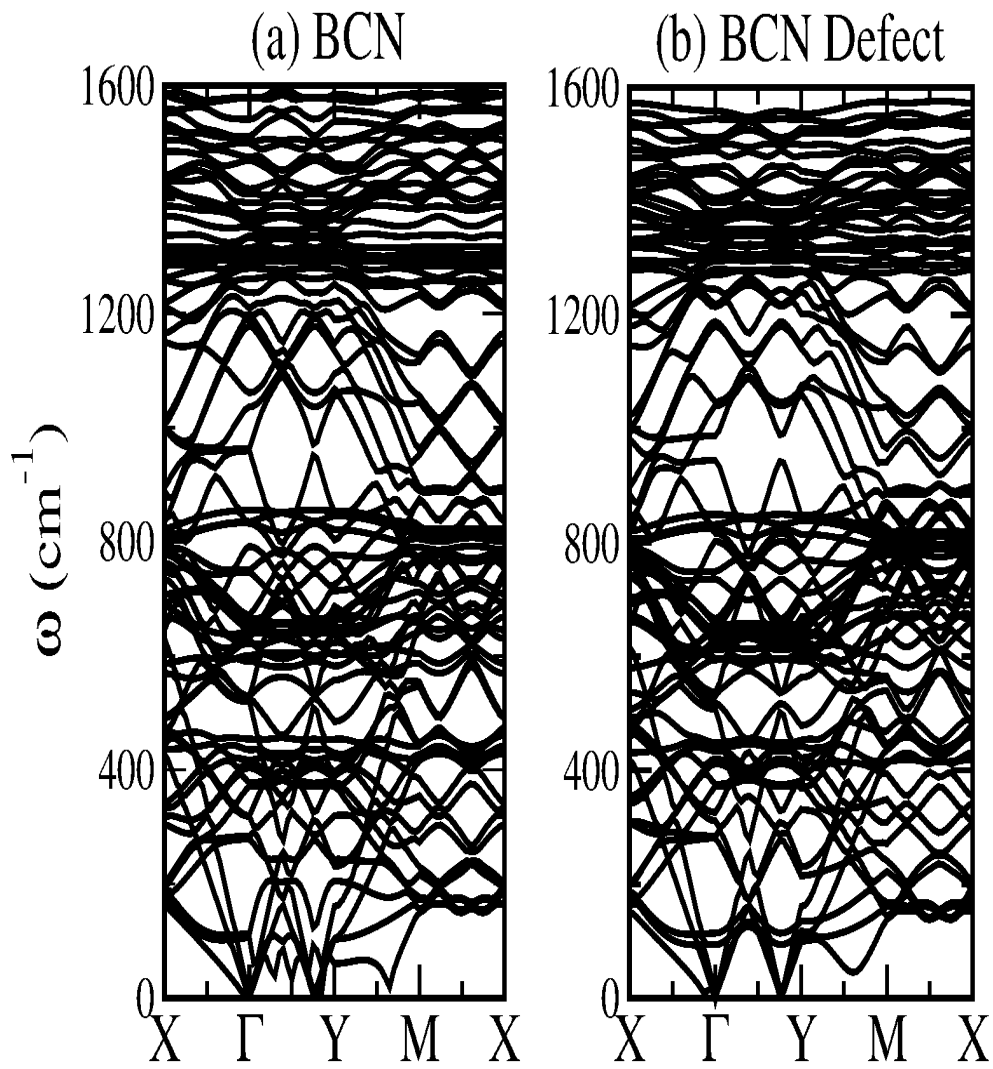


Fig. 6 SI-4: Phonon band structure of BCN monolayers as shown in Figure 1(a,b).

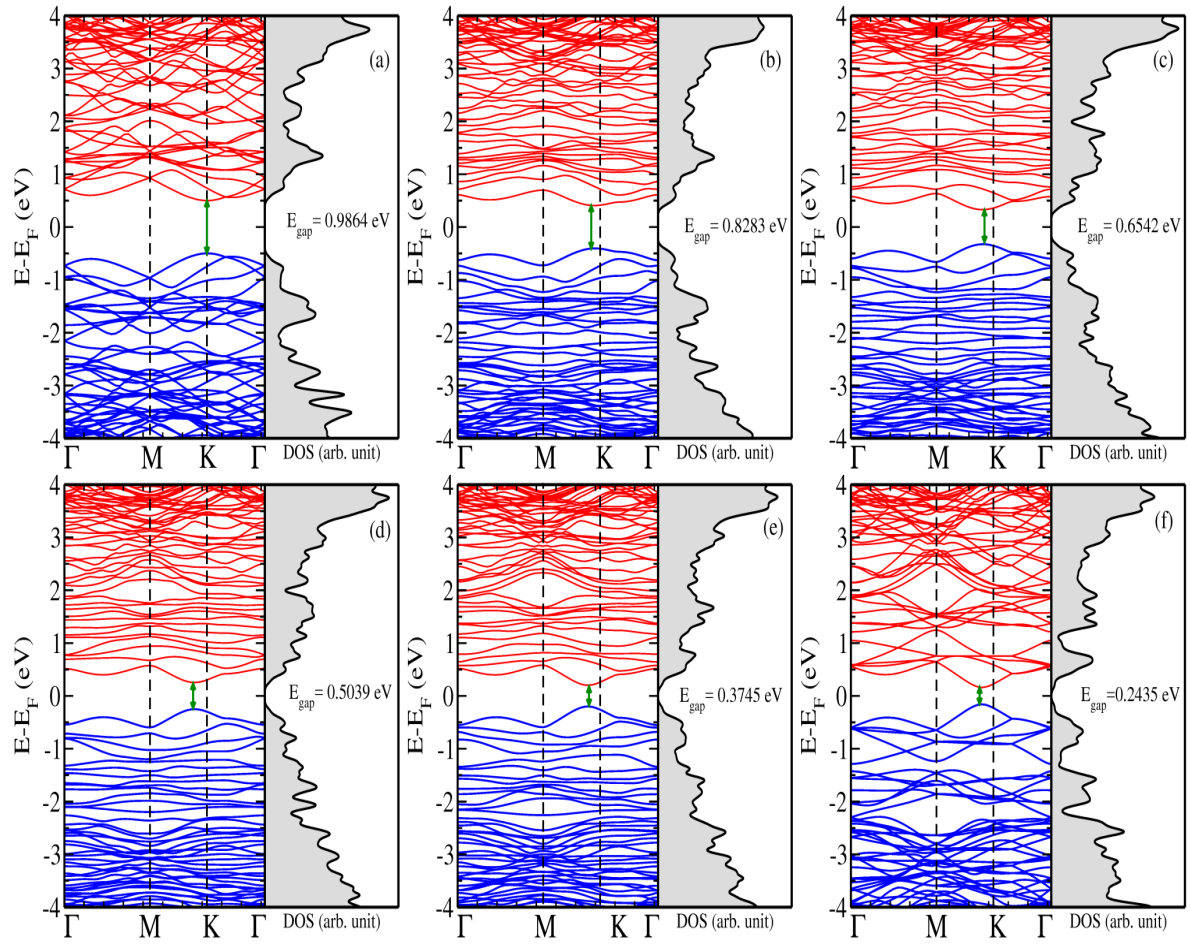


Fig. 7 SI-5: Band Structure and total density of state (TDOS) plot for (a) Fig. 1a, (b) Fig. 7a, (c) Fig. 7b, (d) Fig. 7c, (e) Fig. 7d, and (f) Fig. 1b.

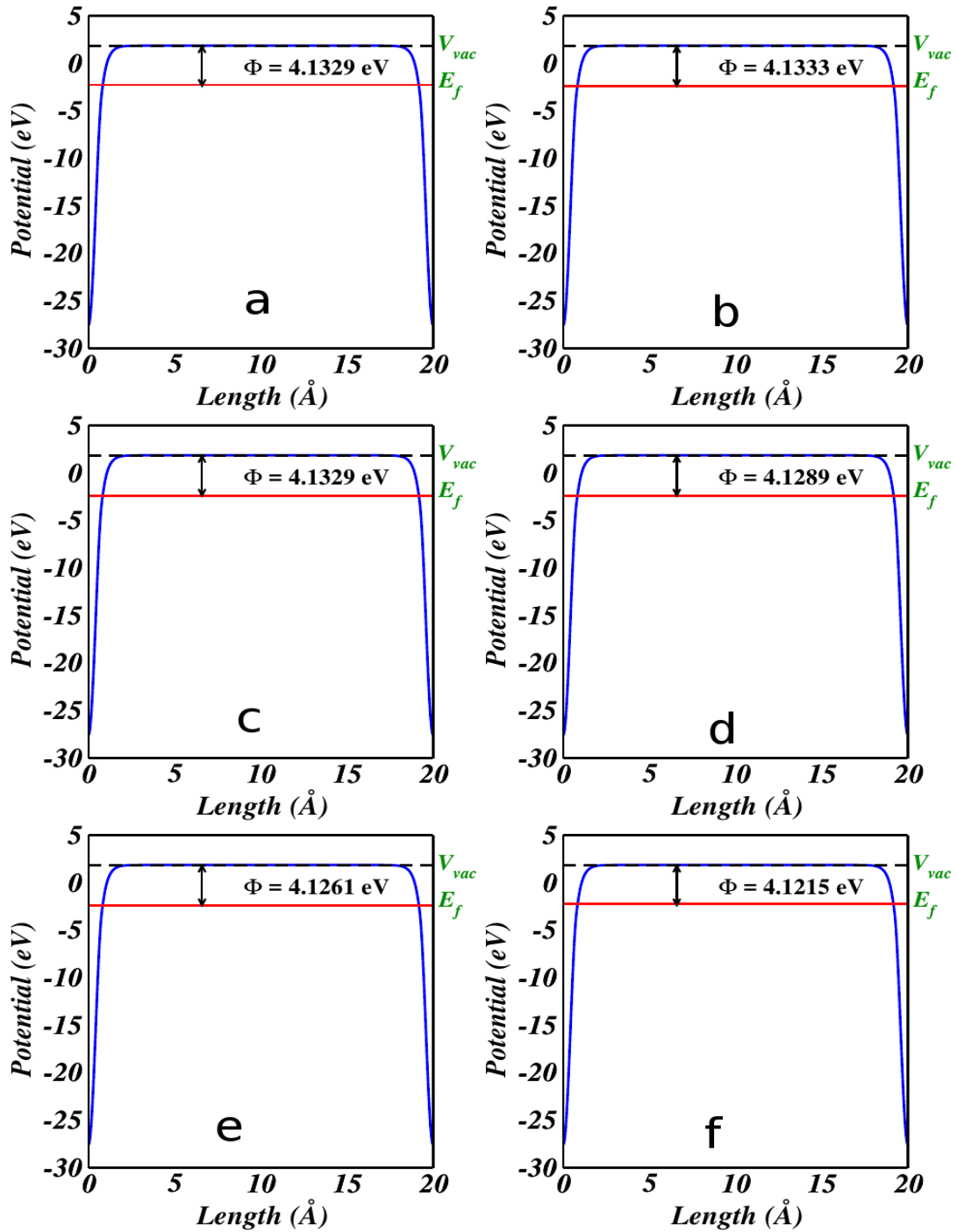


Fig. 8 SI-6: Work function plot for (a) Fig. 1a, (b) Fig. 7a, (c) Fig. 7b, (d) Fig. 7c, (e) Fig. 7d, and (f) Fig. 1b.