Supporting Information

Atomically engineered black phosphorene nanosheets for selective detection of ovarian cancer VOC biomarkers

Ramkumar D[1], Jeeva vergin raj K A, Viveka N, C. Preferencial Kala[1,,] Hariharan R M,*

Centre for Materials Sciences and Nanodevices, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur 603203, India.

(Corresponding author Email: preferec@srmist.edu.in)*

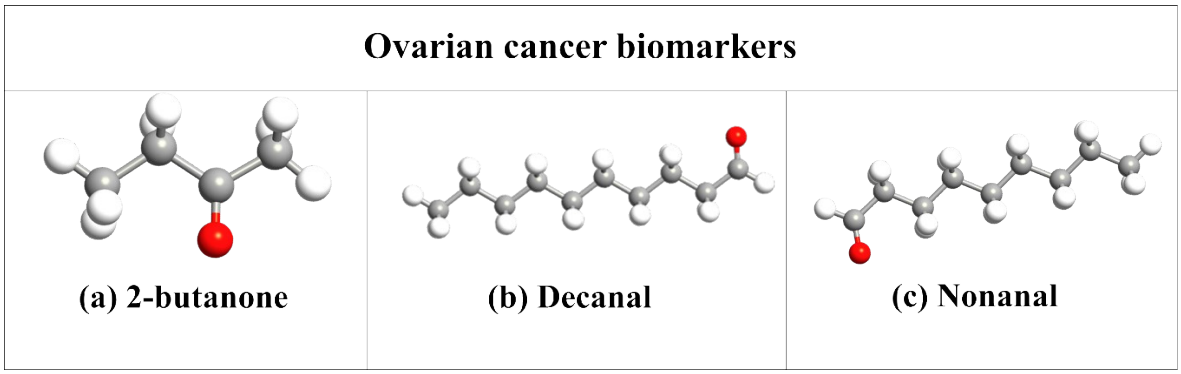

Figure S1: DFT-relaxed free molecular structures of three VOCs, related to ovarian cancer biomarkers: (a) 2-butanone (b) Decanal (c) Nonanal.

Table S1. Calculated adsorption energies (E_{ads}) and equilibrium distances (d) for OC VOCs adsorbed on black phosphorene.

VOC molecule	Adsorption configuration	E_{ads} (eV)	d(Å)
2-butanone	Vertical	-0.10	3.10
	Horizontal	-0.12	3.16
Decanal	Vertical	-0.14	3.00
	Horizontal	-0.45	3.04
Nonanal	Vertical	-0.08	3.06
	Horizontal	-0.13	3.14

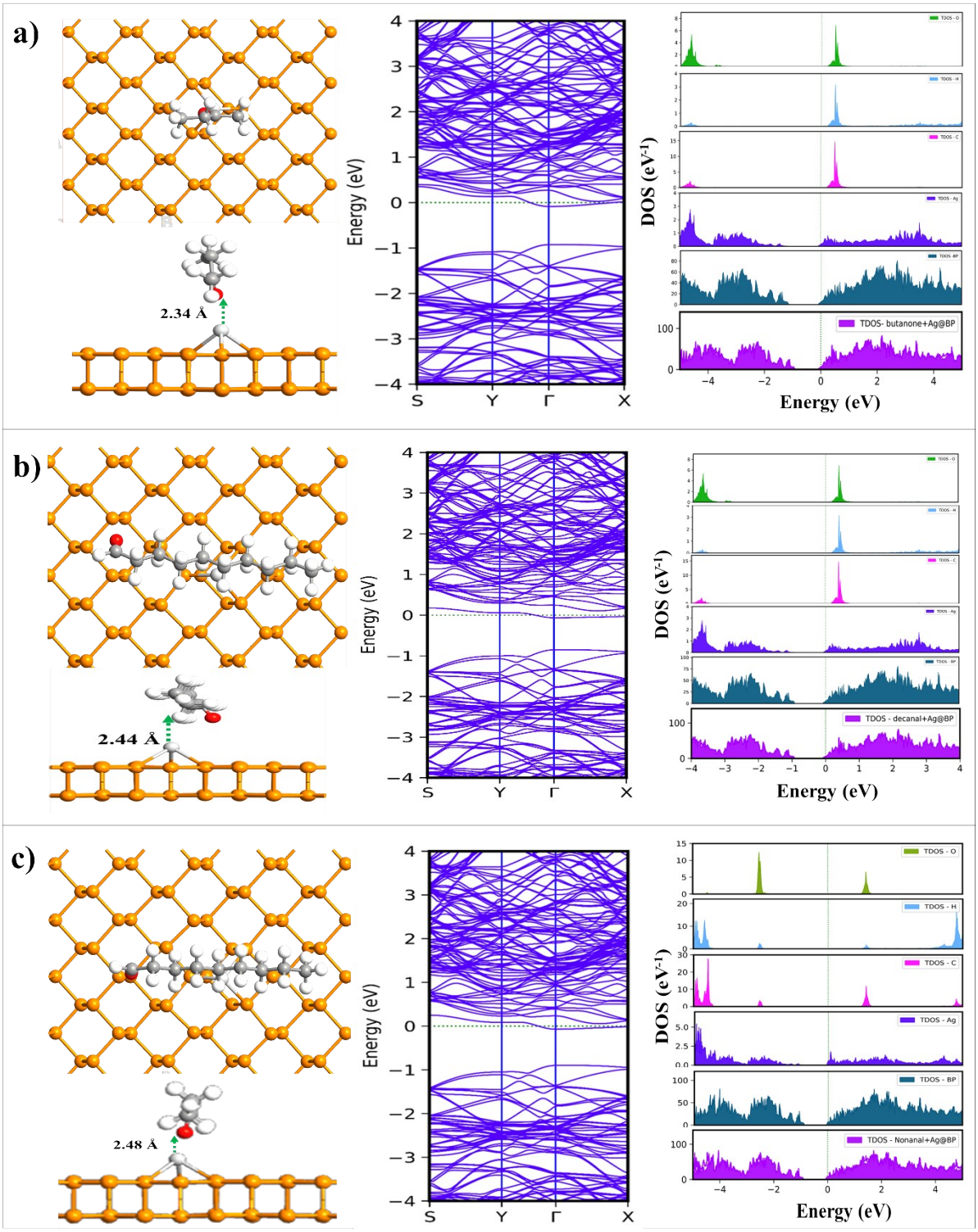

Figure S2. Relaxed structure of three VOCs related to OC biomarkers, on Ag decorated BP (Top and side views) and band structure and projected density of states (PDOS): (a) 2-butanone, (b) decanal, (c) nonanal.

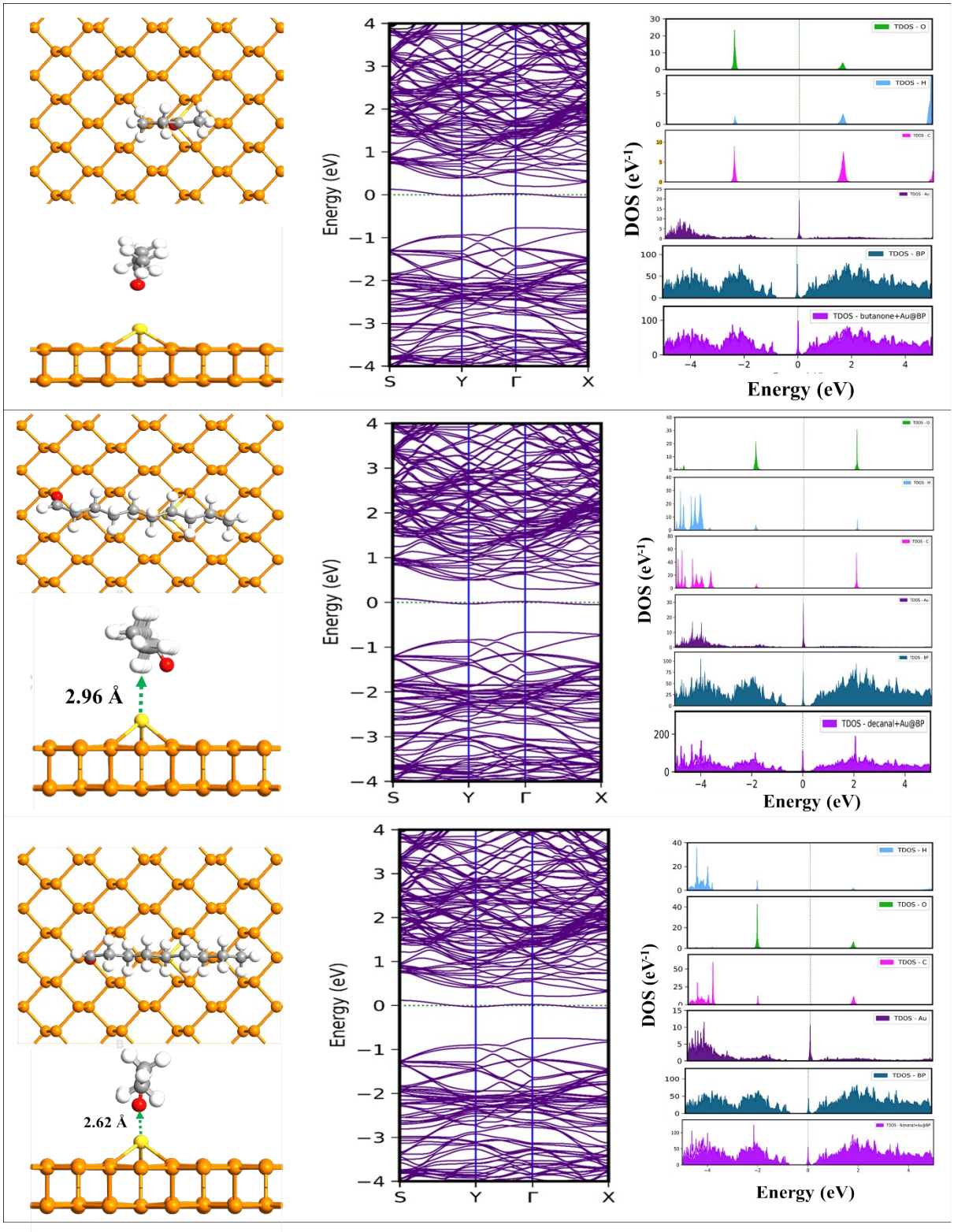

Figure S3. Relaxed structure of three VOCs related to OC biomarkers, on Au decorated BP (Top and side views) and band structure and projected density of states (PDOS): (a) 2-butanone, (b) decanal, (c) nonanal.