Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Charge-Transport Anisotropy in Black Phosphorus: Critical dependence on the number of layers

Swastika Banerjee[a] and Swapan K. Pati*[a, b]

[a.] †New Chemistry Unit, ‡Theoretical Sciences Unit
[b.] Jawaharlal Nehru Center for Advanced Scientific Research
[c.] Jakkur P. O., Bangalore 560064, India
[d.] *E-mail: swapan.jnc@gmail.com

Computational details: We have carried out a SCF calculation with 70×70×1 k-mesh giving rise to a finer k vs. E (k) spectrum. This can capture the Dirac like state at the vicinity of Γ-point which remains intractable even after using a considerable k-grid of 20×20×1 through HSE06 functional. So, we have shown the band-dispersion pattern along the Γ-X band line (see Fig. 2d) with PBE functional after consideration of 70×70×1. We have included this discussion in the supporting information file. We also have mentioned that Fig. 1d is obtained with PBE functional with dense grid.

Supplementary Figures and Table:

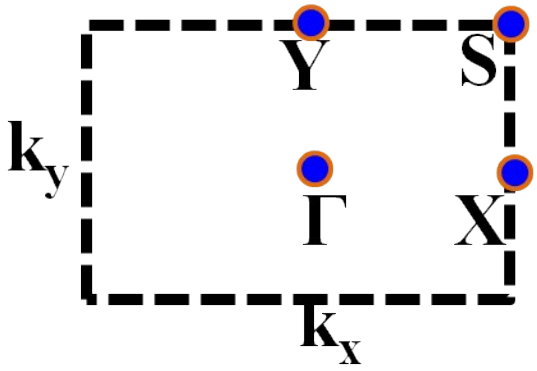

Figure S1. Wigner-Seitz cell with high symmetry k-points is shown for optimized structure of TBP (α-P, ABA stacking) as shown in Figure 1a.

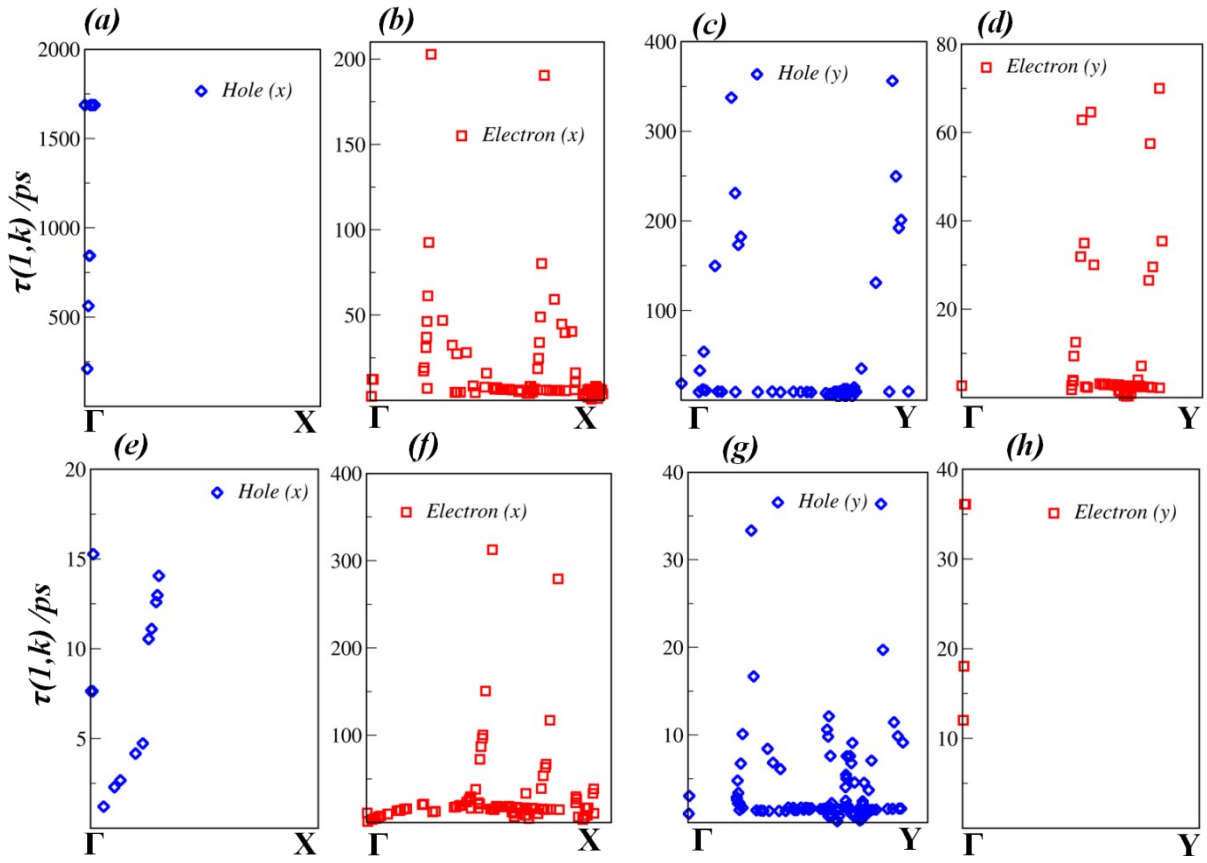

Fig. S2. (a), (b), (c) and (b) represent the plot of relaxation time (as in eq. 2) vs. corresponding carrier-states (in k-space) along different transport direction and carriers for monolayer. (e), (f), (g) and (h) are the same for bulk (black) phosphorous.

Table T1. Carrier types (P), where, $e(h)_{x/y}$ denote electron(hole) transport direction along x/y. Mobilities ($\mu_{effective}$) for monolayer have been calculated using equation (1) at T = 300 K.

P	$\mu_{effective}$ (10^3 $cm^2V^{-1}s^{-1}$)
e_x	0.28
e_y	0.014
h_x	0.57
h_y	12.49