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Optimizing Quantum Capacitance in AsXBr/AsYBr ((X≠Y) = S, Se and Te) Heterostructures for High-Performance Supercapacitors

Himalay Kolavada,[a), b)] Gaushiya A. Shaikh,[b)] P.N. Gajjar,[b),*] and Sanjeev K. Gupta[a), *]

[a)]Computational Materials and Nanoscience Group, Department of Physics and Electronics, St. Xavier's College, Ahmedabad 380009, India

[b)]Department of Physics, University School of Sciences, Gujarat University, Ahmedabad 380009, India

***Corresponding authors**: Dr Sanjeev K. Gupta (E-mail: sanjeev.gupta@sxca.edu.in) and Prof. P. N. Gajjar (E-mail: pngajjar@gujaratuniversity.ac.in)

Supplementary data S1

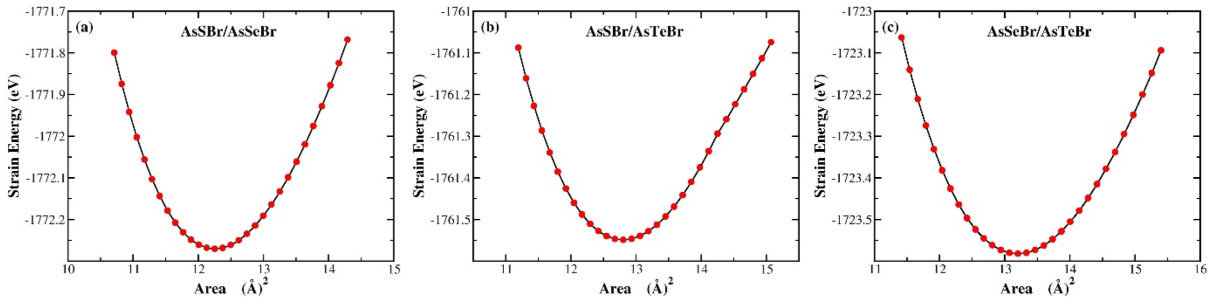

Figure S 1 The change of the total energy with respect to the area of the structures. The continuous curves represent a parabolic fitting of the results, needed to compute the bulk modulus (B).

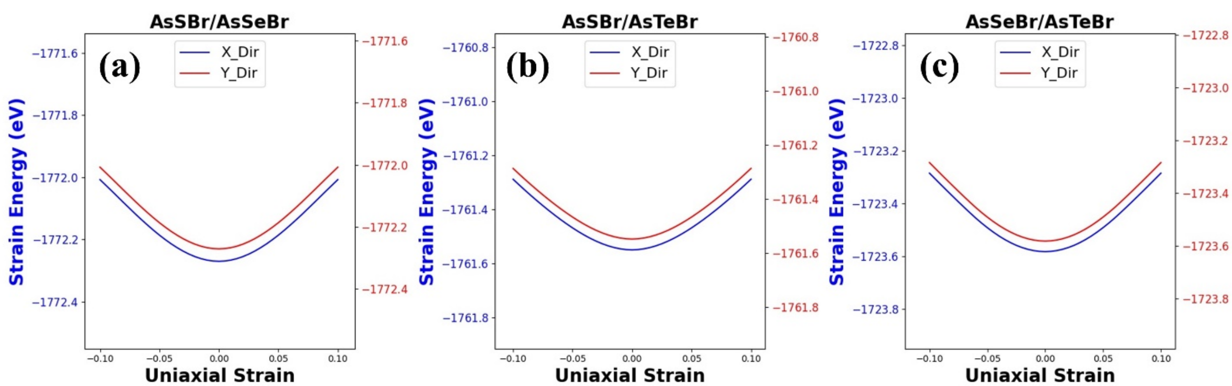

Figure S 2 the change of the total energy with respect to the area of the strain strength along the x and y directions of the AsSBr/AsSeBr, AsSBr/AsTeBr and AsSeBr/AsTeBr structures. The continuous curves are a parabolic fitting of the results, needed to compute Young's modulus (Y).

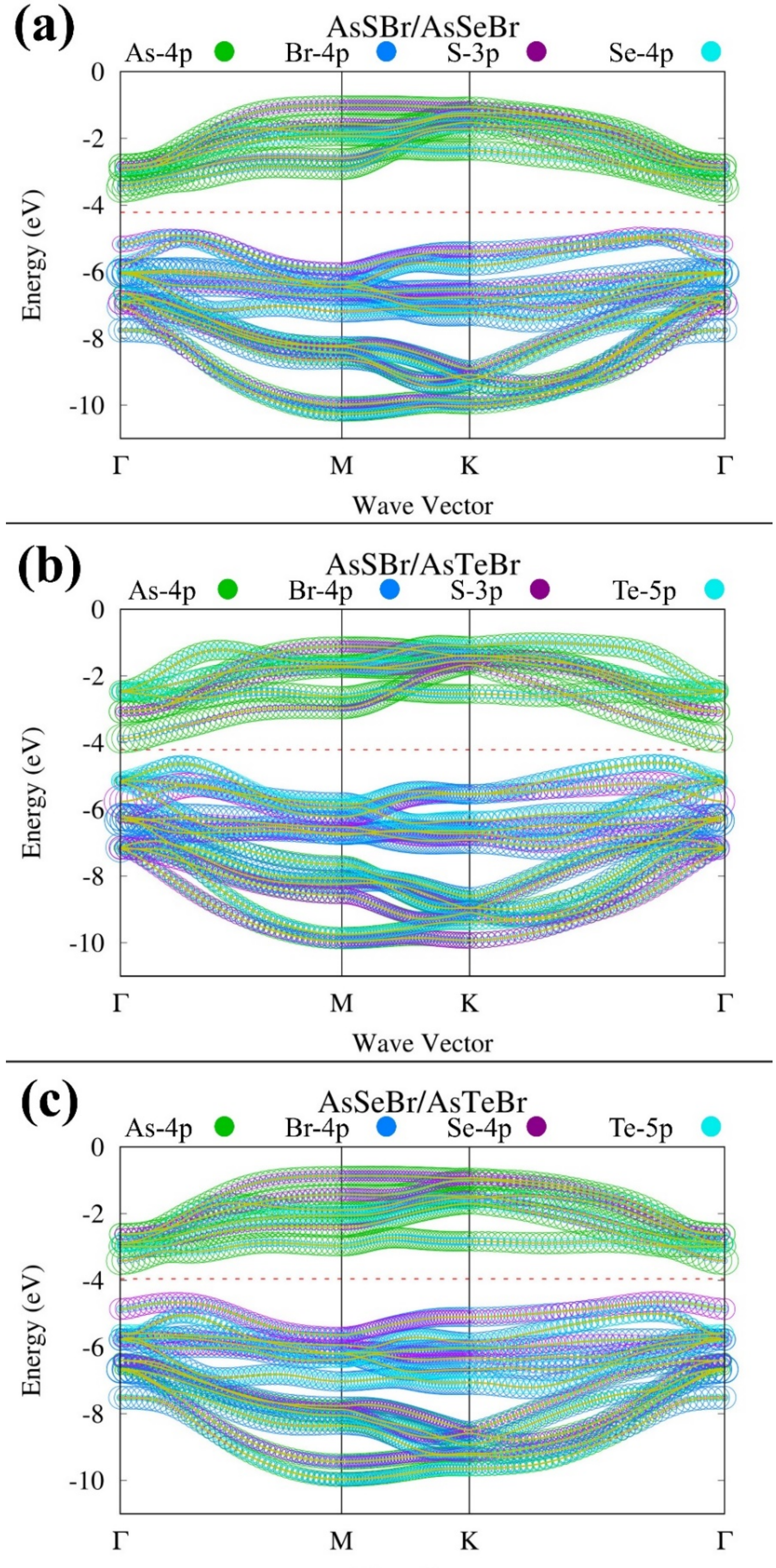

Figure S 3 Illustrating the fatband structures delineating the atom-specific contributions to various electronic bands within the AsSBr/AsSeBr, AsSBr/AsTeBr, and AsSeBr/AsTeBr Janus-heterostructures.

Table S 1 Displaying bandgap, maximum quantum capacitance with applied voltage, maximum charge storage for cathode and anode, along with electrode type suggestions

Janus heterostructure	Bandgap eV	Type of bandgap	CQ-max µF/cm2	Applied voltage V	Qcathode µC/cm2	Qanode µC/cm2	Qcathode/Qanode	Electrode type
AsSeBr/AsSBr	0.82	Indirect	302.66	1	114.53	77.27	1.48	Cathode
AsTeBr/AsSBr	0.27	Indirect	383.40	-1	192.99	132.64	1.46	Cathode
AsTeBr/AsSeBr	0.35	Indirect	393.89	-1	194.28	104.56	1.86	Cathode

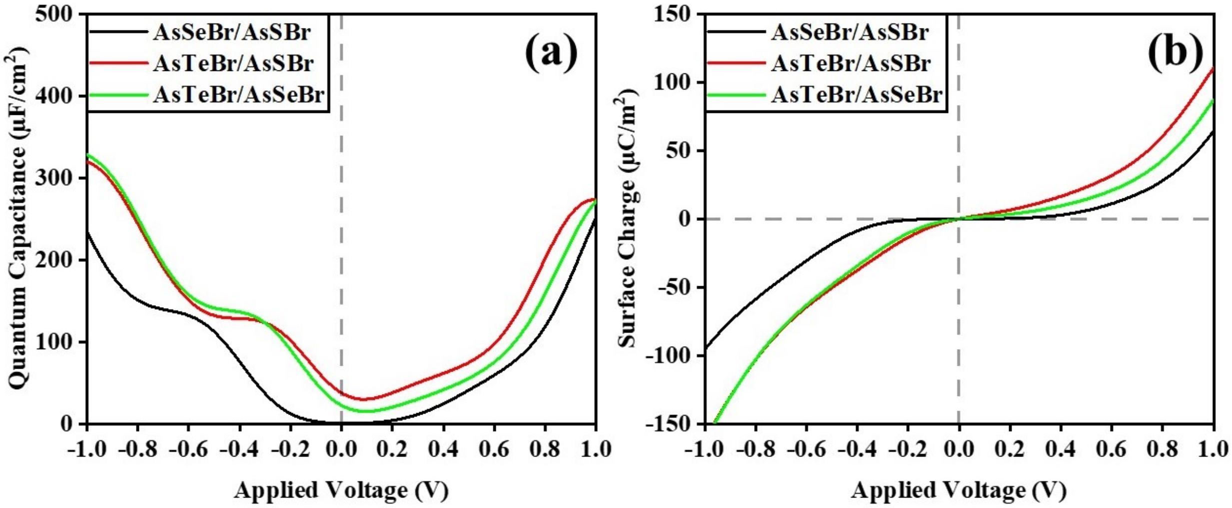

Figure S 4 (a) shows the quantum capacitance and (b) indicate the surface charge with respect to applied voltage for AsSeBr/AsSBr, AsTeBr/AsSBr and AsTeBr/AsSeBr flipped Janus-heterostructures

We also investigated the flipped structure of the reported Janus heterostructures, namely AsSeBr/AsSBr (Se/S), AsTeBr/AsSBr (Te/S), and AsTeBr/AsSeBr (Te/Se). In these flipped structures, the bandgap is reduced compared to the original Janus heterostructures, namely AsSBr/AsSeBr (S/Se), AsSBr/AsTeBr (S/Te), and AsSeBr/AsTeBr (Se/Te). The reduction in bandgap is observed to be 0.82 eV, 0.27 eV, and 0.35 eV for Se/S, Te/S, and Te/Se, respectively. Table 1 presents the bandgap, maximum quantum capacitance ($C_{Q\text{-}max}$), maximum charge storage on the cathode and anode sides, and the type of electrode for each flipped heterostructure.

Furthermore, Supplementary Figure S4 illustrates the quantum capacitance and surface charge of the flipped heterostructures. It is observed that due to the higher density at the Fermi region, the CQ increases compared to the reported structures. Specifically, the maximum C_Q for Se/S is 302.66 µF/cm² at +1.0 V, which is 29.05% lower than that of S/Se. Similarly, for Te/S and Te/Se, the $C_{Q\text{-}max}$ values are 383.40 µF/cm² and 393.89 µF/cm² at -1.0 V, respectively. Interestingly, the CQ-max for Te/S is 10.86% lower than that of S/Te, while for Te/Se, it is 26.63% lower than that of Se/Te. These results suggest that the original Janus-hetero structures are more suitable as electrode materials for supercapacitors.

Moreover, it is noteworthy that the charge storage on the cathode side is higher than that on the anode side for these flipped Janus heterostructures, indicating a cathode nature similar to that of the original Janus heterostructures.