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

BlueP Encapsulated Janus MoSSe as Promising Heterostructure Anode Materials for LIBs

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Fig. S1: (i) Phonon dispersion spectra of various stacking configurations of BlueP-SMoSe heterostructure. (a) All P atoms above Mo and S atoms (b) All P atoms above S atoms. (c) All P atoms above Mo atoms.

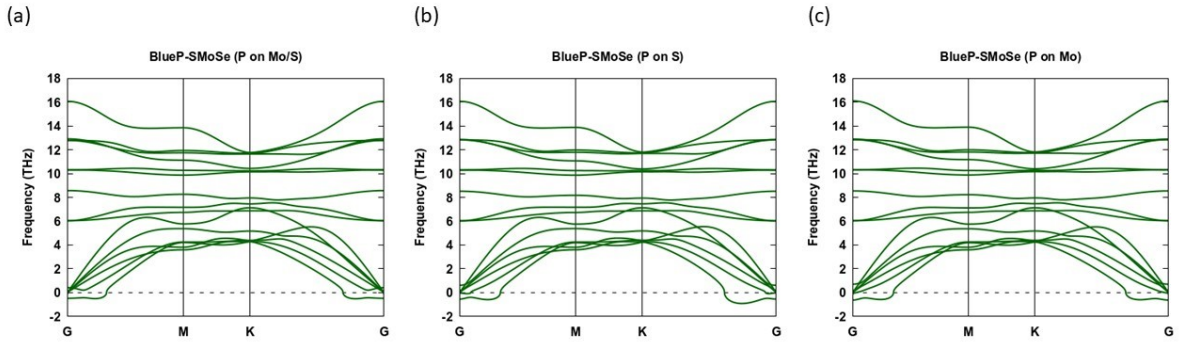

Fig. S1: (ii) Phonon dispersion spectra of various stacking configurations of BlueP-SeMoS heterostructure. (a) All P atoms above Mo and Se atoms (b) All P atoms above Se atoms (c) All P atoms above Mo atoms.

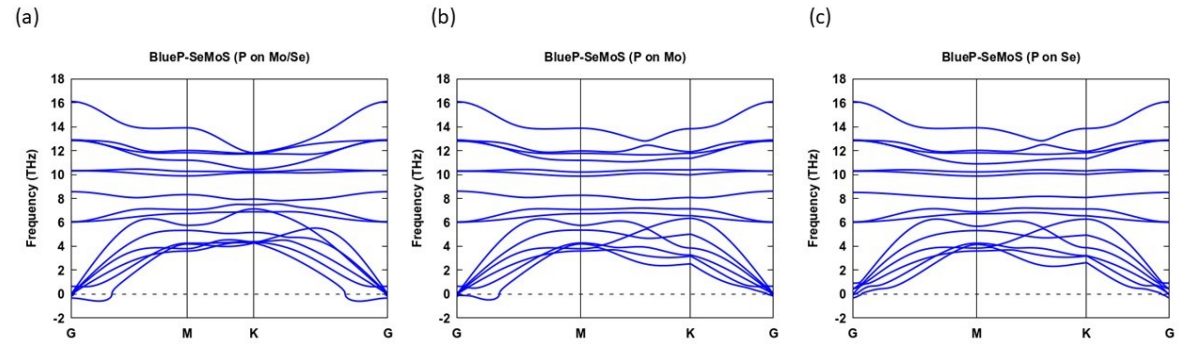

Fig. S2 (i): Variation of total energy with applied (a) uniaxial strain along the x-axis, (b) uniaxial strain along the y-axis, and (c) bi-biaxial strain along the x and y-axis for lithiated BlueP-SMoSe heterostructure.

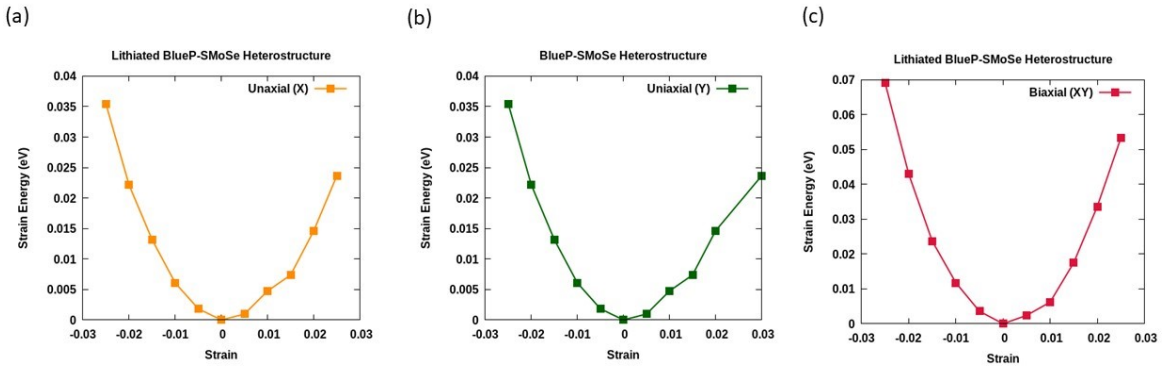

Fig. S2 (ii): Variation of total energy with applied (a) uniaxial strain along the x-axis, (b) uniaxial strain along the y-axis, and (c) bi-biaxial strain along the x and y-axis for lithiated BlueP-SeMoS heterostructure.

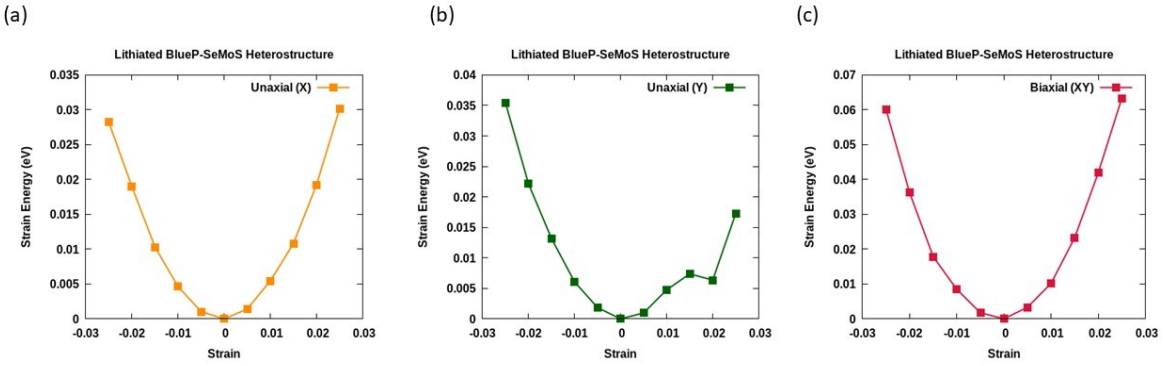

Table S1: The calculated Li diffusion energy when Li migrates at various surfaces and interfaces of BlueP-Janus MoSSe heterostructures from one stable adsorption location to another.

BlueP-SMoSe Heterostructure		BlueP-SeMoS Heterostructure	
Surface	Barrier Energy (eV)	Surface	Barrier Energy (eV)
Li-BlueP-SMoSe	0.085	Li-BlueP-SeMoS	0.081
BlueP-Li-SMoSe	0.221	BlueP-Li-SeMoS	0.135

BlueP-SMoSe-Li	0.166	BlueP-SeMoS-Li	0.188

Table S2: The calculated Li diffusion coefficient when Li migrates at various surfaces and interfaces of BlueP-Janus MoSSe heterostructures from one stable adsorption location to another.

BlueP-SMoSe Heterostructure		BlueP-SeMoS Heterostructure	
Surface	Diffusion Co-efficient (cm^2/sec)	Surface	Diffusion Co-efficient (cm^2/sec)
Li-BlueP-SMoSe	6.05×10^{-5}	Li-BlueP-SeMoS	7.06×10^{-5}
BlueP-Li-SMoSe	3.16×10^{-7}	BlueP-Li-SeMoS	8.78×10^{-6}
BlueP-SMoSe-Li	2.66×10^{-6}	BlueP-SeMoS-Li	2.99×10^{-8}