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

Supplementary Materials for

Interfacial Effects on Lithium-ion Diffusion in Two-dimensional Lateral Black Phosphorus–Graphene Heterostructures

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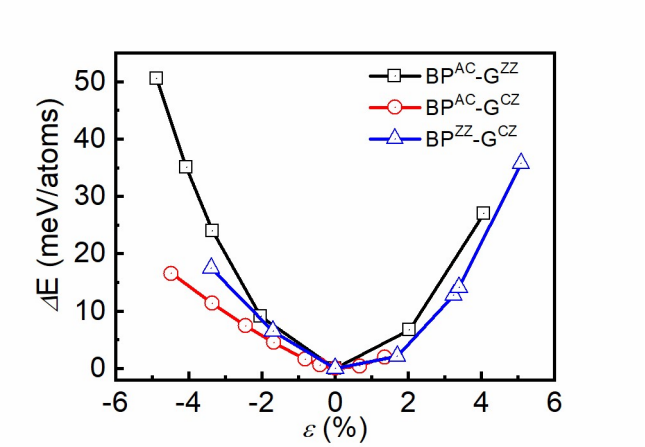

Figure S1. Total Energy differences (ΔE) with compress or tensile strain (ε) in the *y* direction for BP^{AC}-G^{ZZ}, BP^{AC}-G^{CZ} and BP^{ZZ}-G^{CZ} heterostructures.

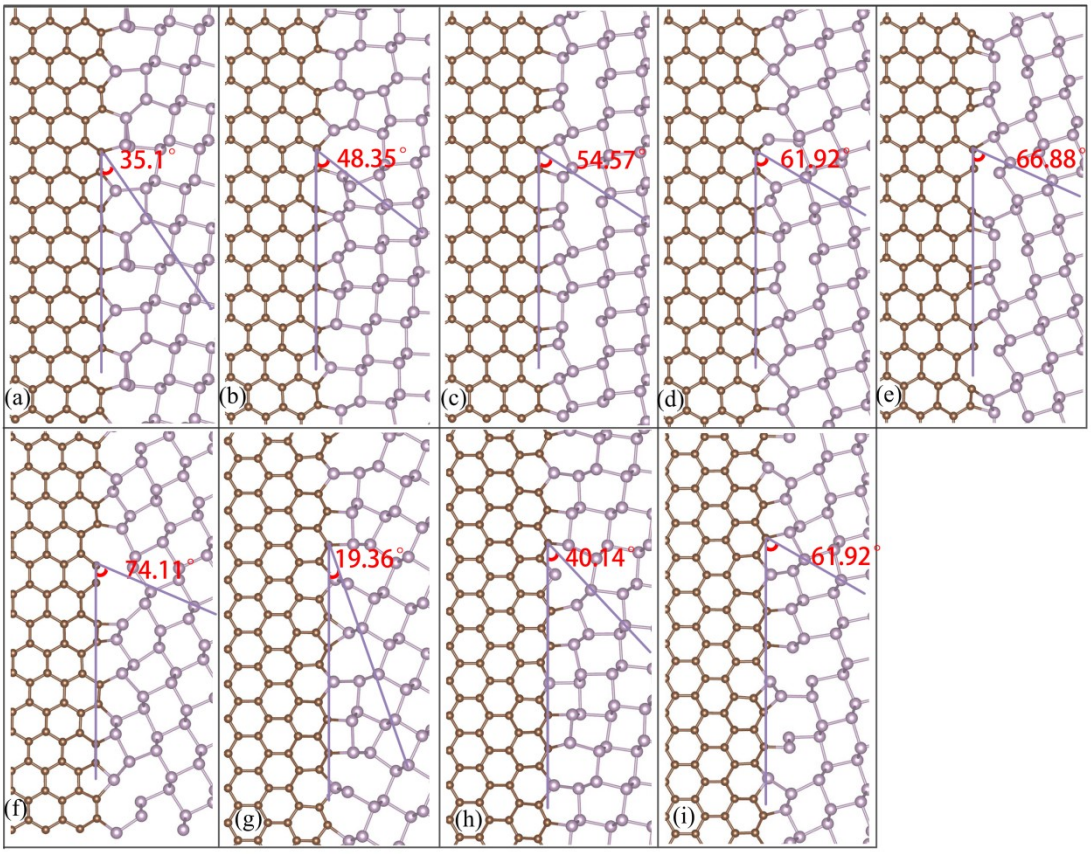

Figure S2. Atomic interfacial structures obtained for all the other stable BP^{R}–G heterostructures with AC (a–f) and ZZ (g–i) edge of graphene domain. Rotation angles of the BP domains are labelled in red.

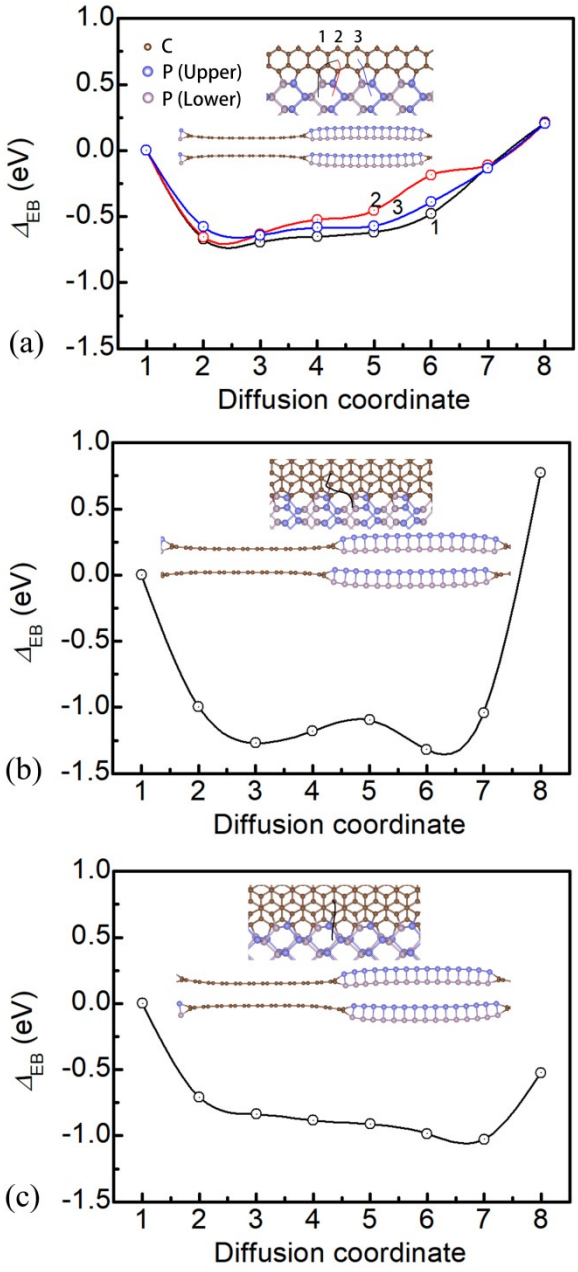

Figure S3. Li-ion diffusion paths and the corresponding Δ_{EB} values obtained for (a) AA-stacking, (b) AB-stacking and (c) shifted AB-stacking crystal structure of BP^{AC}-G^{ZZ}.