Supporting information

Enhanced Sodium-Ion Intercalation and Migration in C/B-Doped WS₂/Graphene Bilayers: Insights from Electronic Structure Calculations

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Figure S1. Optimized geometric structures of the 4:5 WS₂/G with top and side views.



Figure S2. Optimized geometric structures of the 4:5 B/C-dopped WS₂/G with top and side views (a)/(b).



Figure S3. Geometric structures of B/C-dopped WS₂/G upon intercalation of 6 Na ions on the surface (a/b) and within interfacial space (c/d) with top view.