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Boosted Lithium-ion hopping on halogen-doped χ_3 borophene

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Figure S1

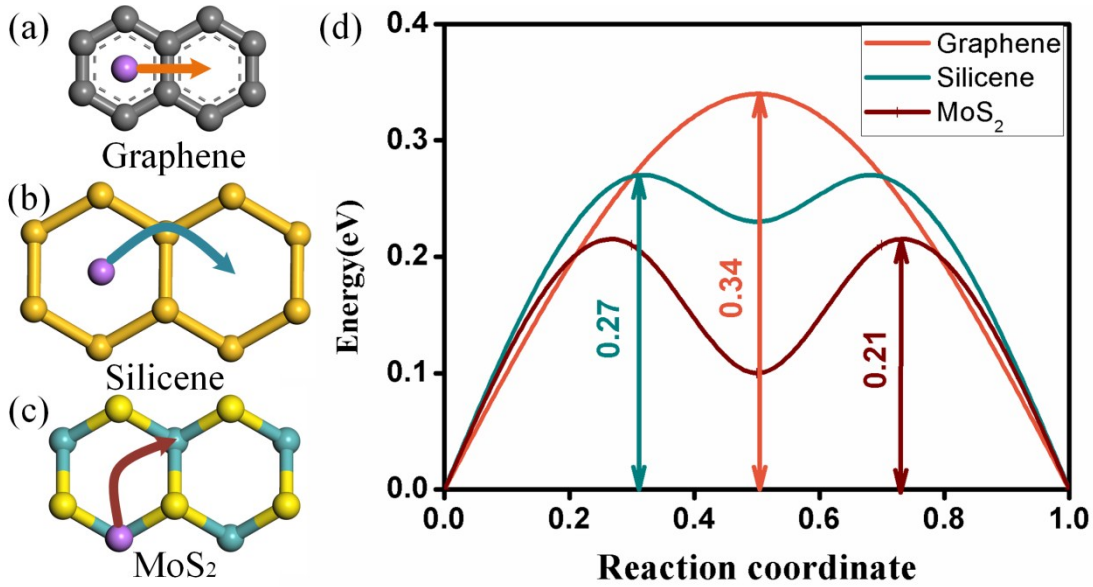

Figure S1. Schematic illustration of Li-ion migration pathways on 4 × 4 supercell (a) graphene, (b) silicene and (c) MoS_2 and (d) the corresponding energy profiles.

Figure S2

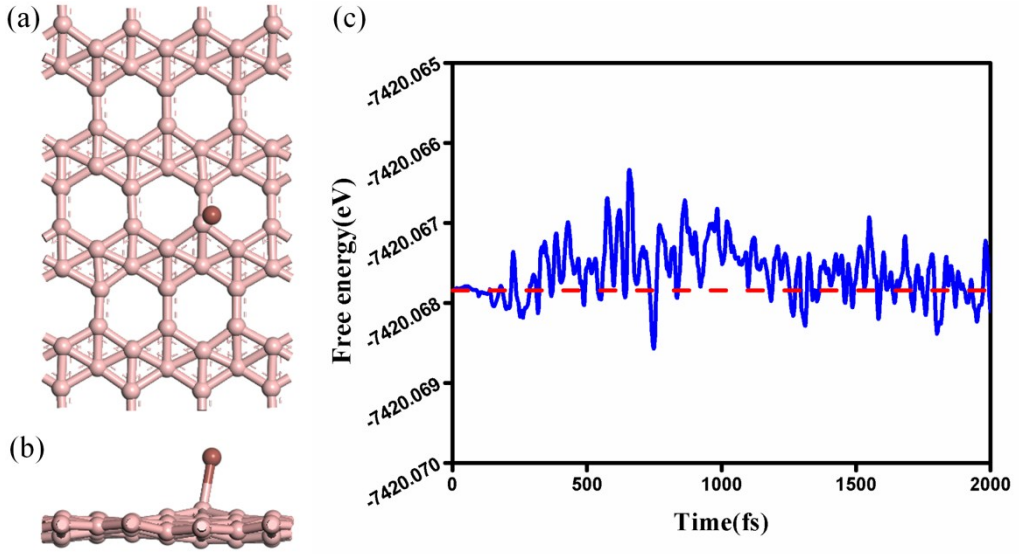

Figure S2. (a) Top and (b) side views of I-doped χ_3 borophene obtained at the end of the simulation performed at 300 K. (c) Evolution of the free energy versus simulation time.