Supplementary Materials

Unraveling the Interactions between Lithium and Twisted Graphene

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The potential energy profiles of Li and Li^+ referring to t-BLG were evaluated for slab-Li/Li+ distances up to 6 Å considering three symmetry adsorption sites (Top, Hollow, Bridge) and outside configuration. The potential energies plots are shown in Figure1S

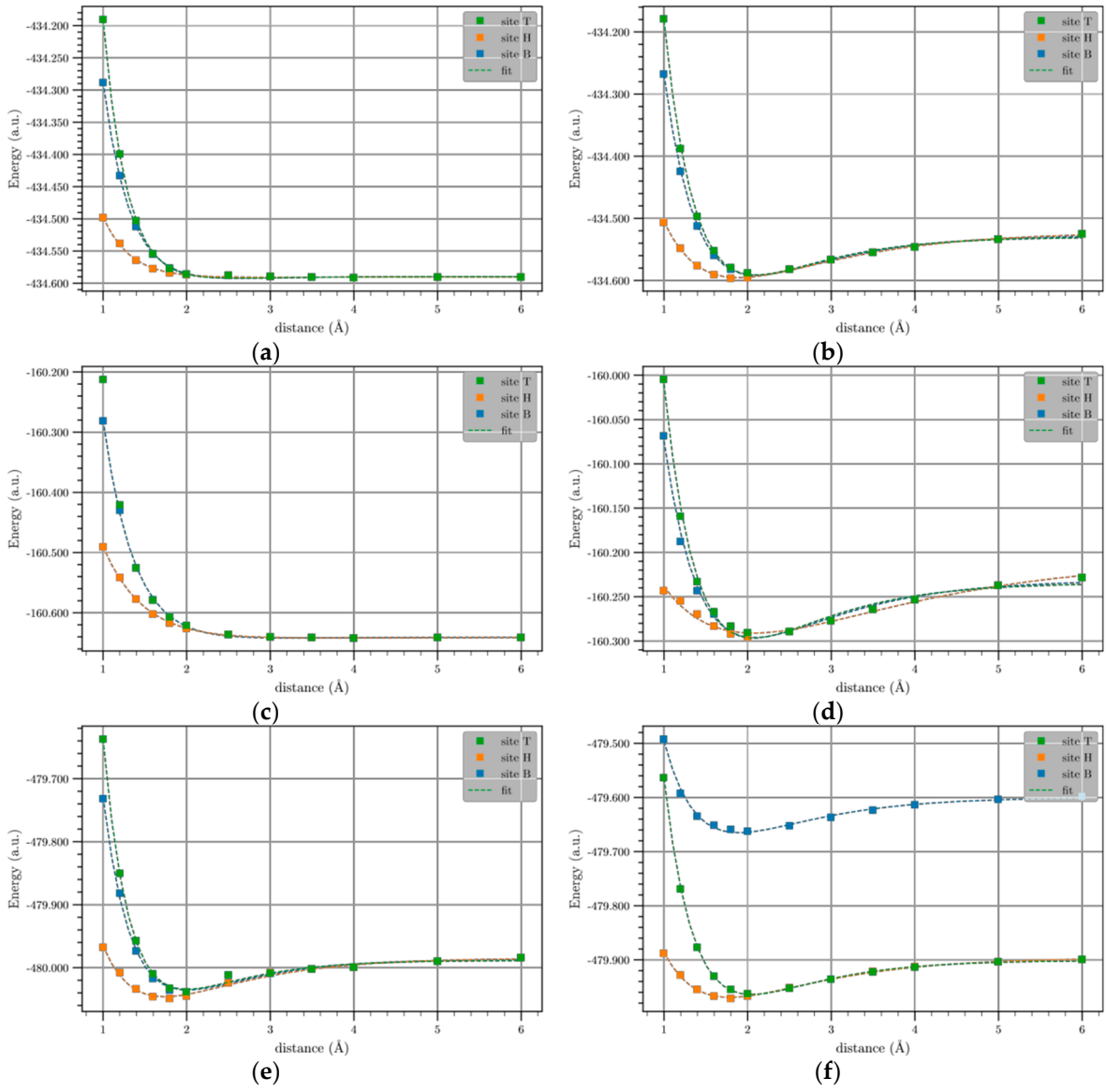

Figure S1. The potential energy profiles of Li (a), (c), (e) and Li^+ (b), (d), (f) for twist angles of 13.17°, 21.79°, 38.21° respectively, outside configuration.

The potential energy profiles of Li and Li^+ referring to t-BLG were evaluated for interlayer distances up to 6 Å considering three adsorption sites and inside configuration. The potential energies plots are shown in Figure S2

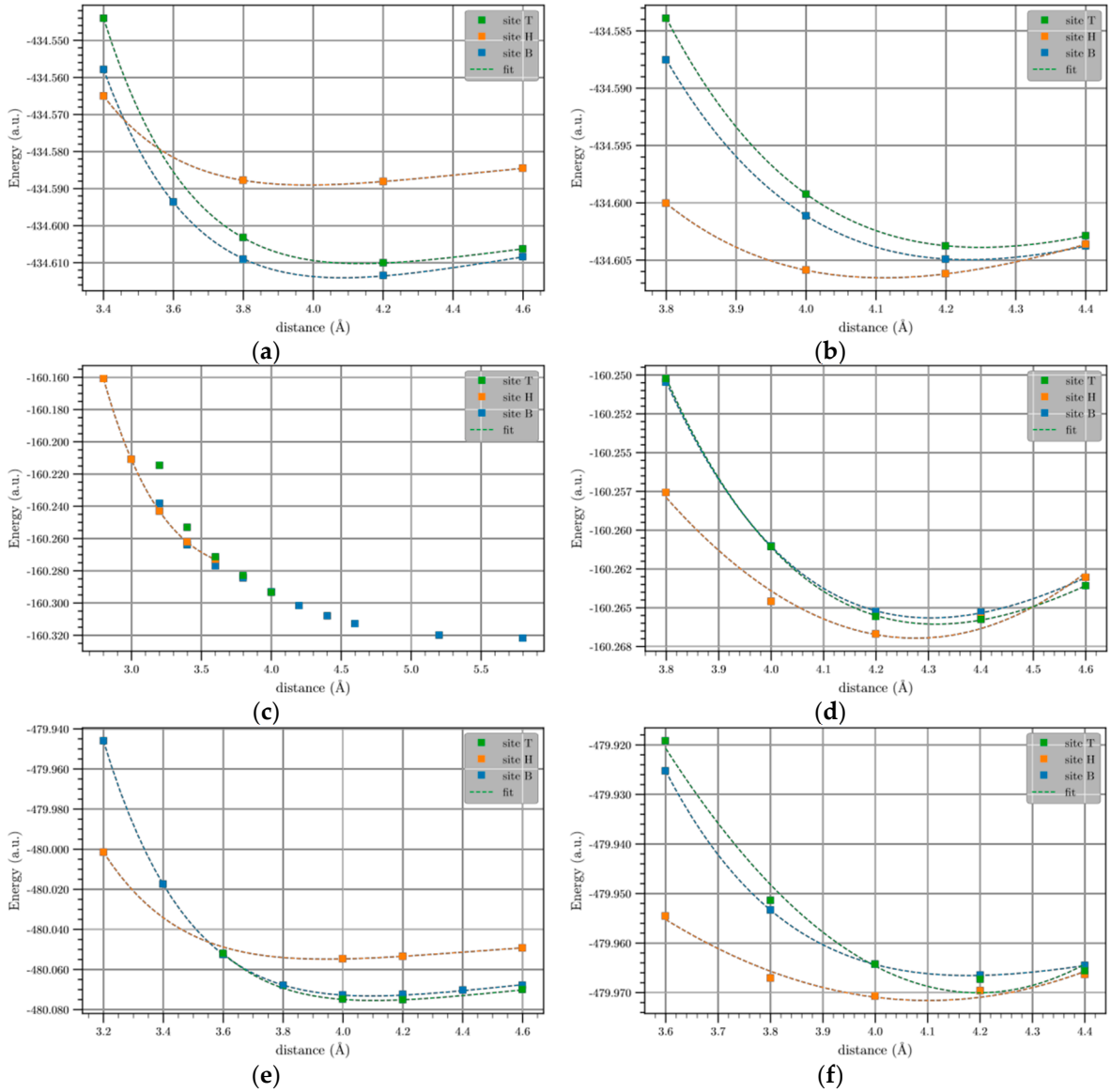

Figure S2. Potential energy profiles of Li (a), (c), (e) and Li^+ (b), (d), (f) for twist angles of 13.17°, 21.79°, 38.21°, respectively, considering inside configuration (sandwich).