Unblocking the potential of a Novel 2D Vanadium Boro Carbide and VBC/graphene heterostructure as an Efficient Host for Li-Ion Batteries

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Supporting Information

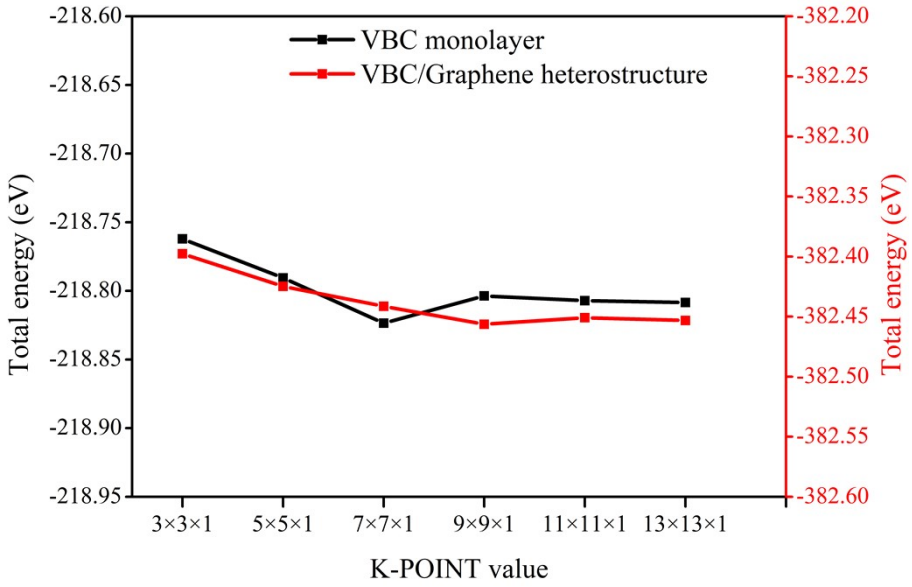

Figure 1. K-point value versus total energy of the VBC monolayer and VBC/graphene heterostructure.

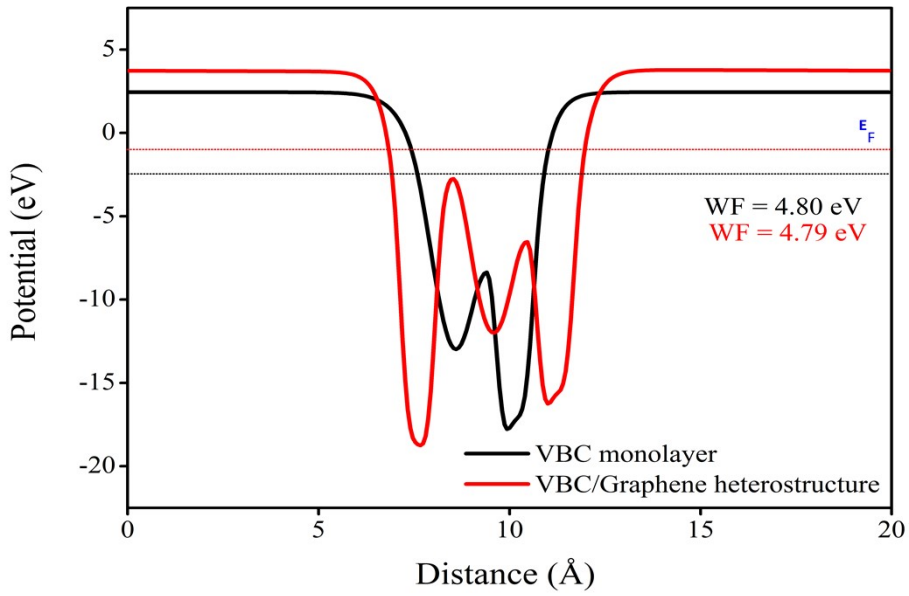

Figure 2. Work function of the pristine VBC monolayer and VBC/graphene heterostructure.

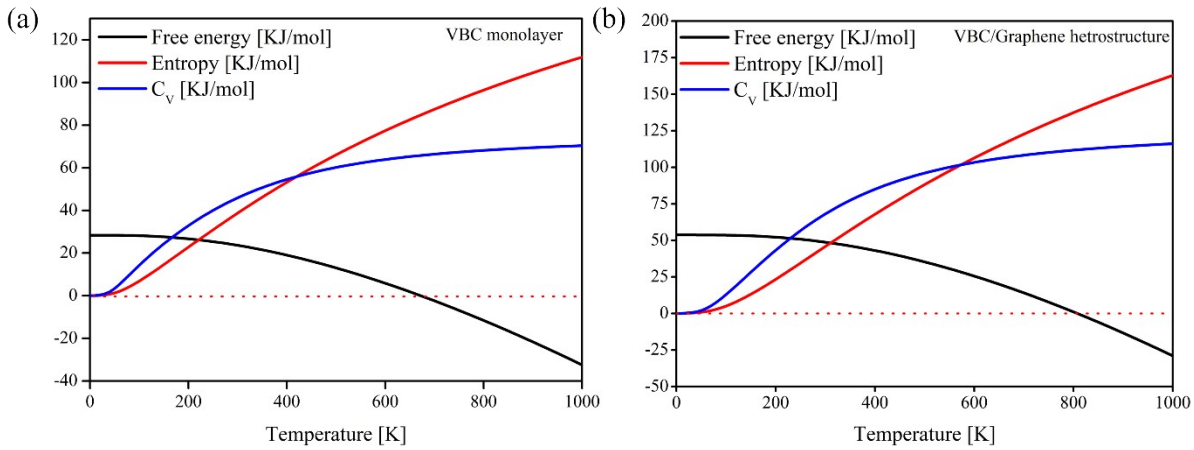

Figure 3. Thermodynamic quantities: Gibbs free energy (F), entropy, and heat capacity at constant volume (C_v) as functions of temperature (K) of the VBC monolayer and VBC/graphene heterostructure.

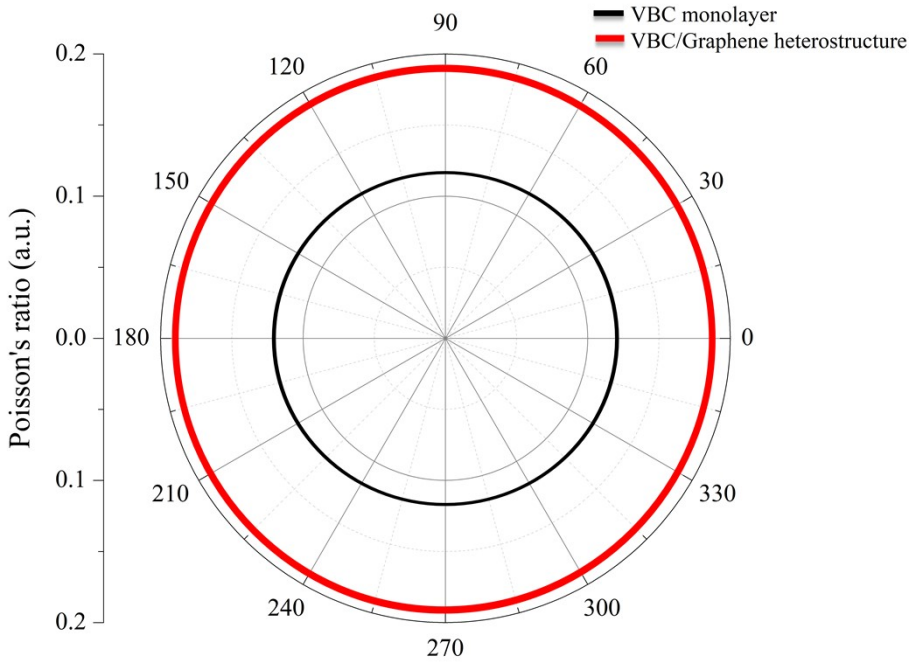

Figure 4. Poisson's ratio of the VBC monolayer and VBC/graphene heterostructure.

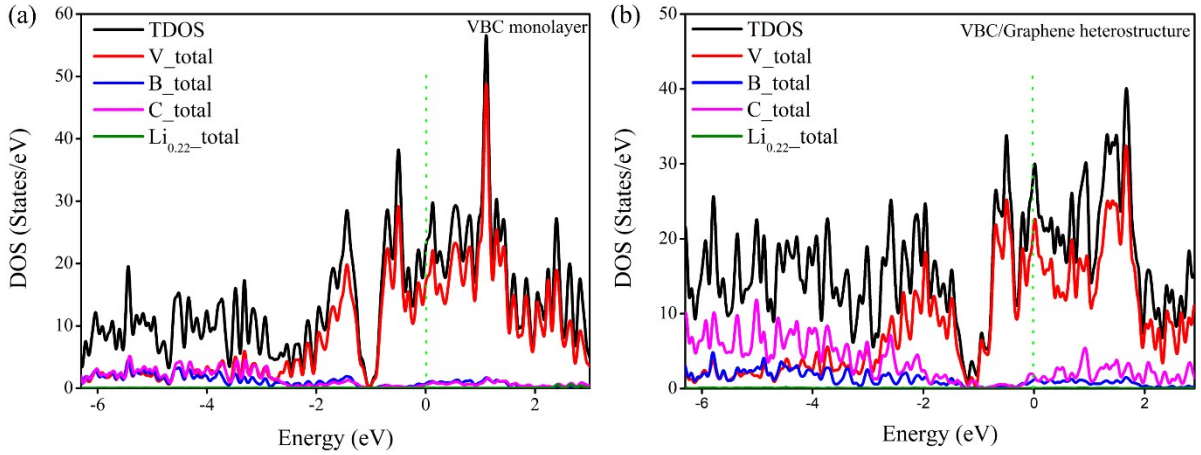

Figure 5. Total and partial density of state of the Li-adsorbed VBC monolayer and VBC/graphene heterostructure.

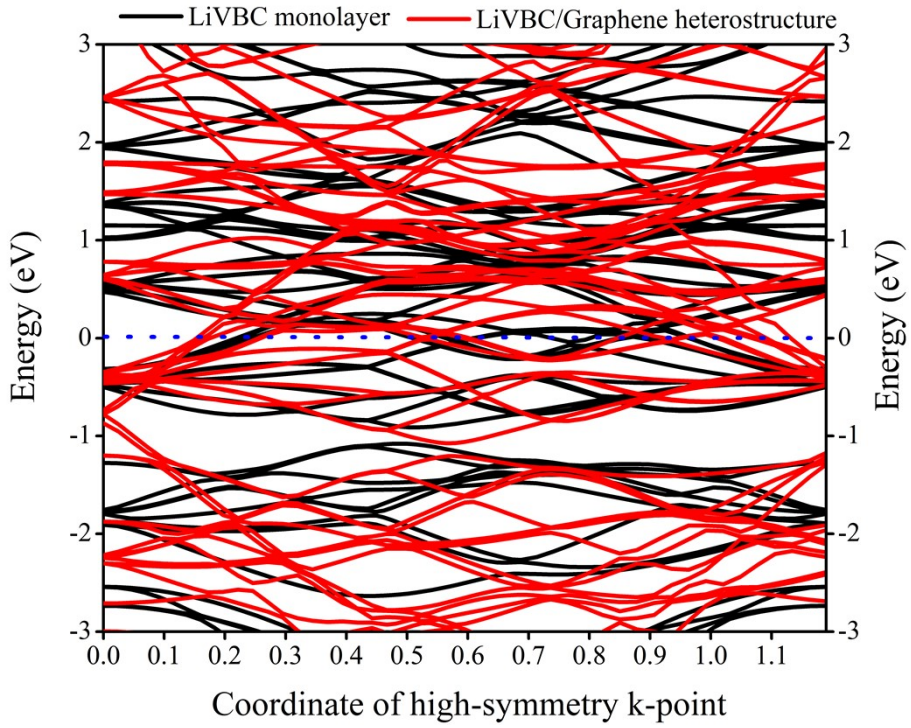

Figure 6. Electronic band structure of the Li-adsorbed VBC monolayer and VBC/graphene heterostructure.

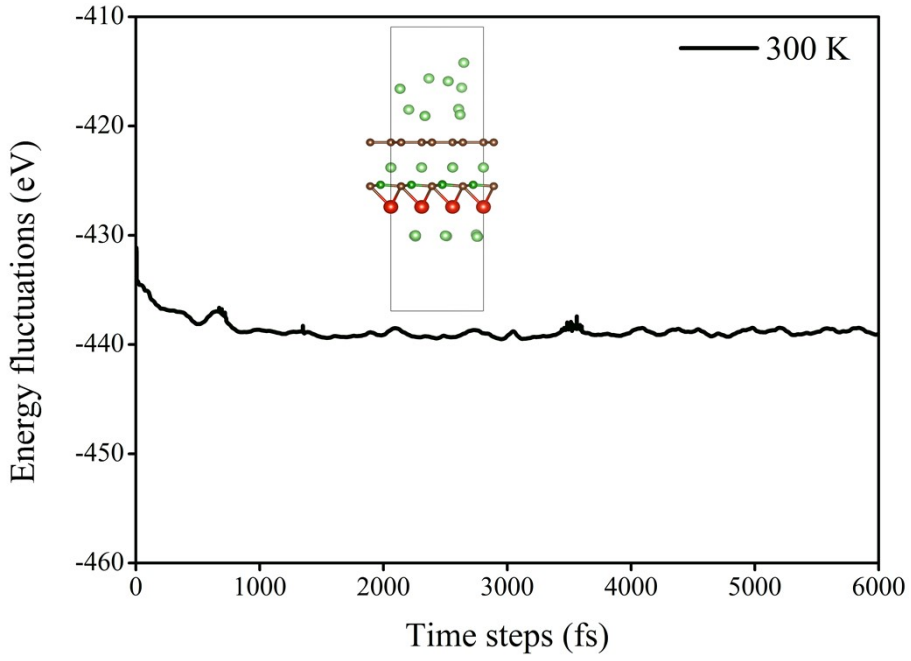

Figure 7. AIMD simulations of the VBC/graphene heterostructure at 300 K.

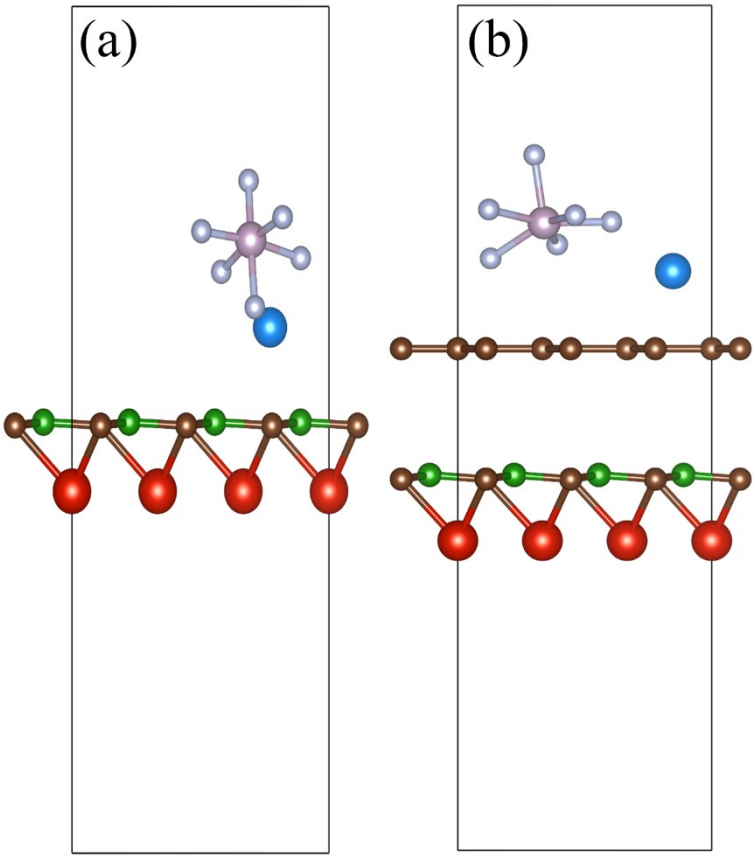

Figure 8. The most favourable adsorption configuration of the (a) VBC monolayer and (b) VBC/graphene heterostructure with adsorbed $LiPF_6$.