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Density functional theory study on zigzag and armchair nanotubes of AlP for potential K-ion battery application

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Abstract

The B3LYP-gCP-D3/6-31G* model was employed to explore the potential use of armchair AlP nanotube (A-AlPNT) and zigzag Z-AlPNT as anode materials for use in K-ion batteries (KIBs). The adhesion energy of K^+ on the A-AlPNT or Z-AlPNT was found to be −46.6 or −43.1 kcal/mol, while the interaction with K atoms was weaker with an adhesion energy of −5.3 or −4.7 kcal/mol, respectively. The dispersion term was more crucial for K atom interaction than the adhesion of K^+, contributing 63.1 and 4.1% to the adsorption energy on Z-AlPNT, respectively. The cell voltage and maximum energy barrier for the migration of K^+ were 1.67 V and 11.3 kcal/mol for Z-AlPNT and 1.79 V and 10.7 kcal/mol for A-AlPNT, respectively. This indicates that AlPNTs have excellent ion mobility with low energy barriers, which enable faster charge/discharge rates. The higher cell voltage and greater ion mobility suggest that A-AlPNTs are promising anode materials for KIBs when compared to Z-AlPNTs. We have also discussed the impact of K/K^+ adsorption on the electronic properties of AlPNTs.