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Abstract	The development of high-performance anode materials is crucial for advancing next-generation ion batteries. Here, we demonstrate cyclic[3]anthracene (C[3]A) as a high-performance anode material for Li/K-ion batteries through DFT calculations. Our results demonstrate that C[3]A exhibits exceptional structural stability, strong Li/K adsorption (binding energies up to −1.52 eV for Li and − 1.42 eV for K), and significant charge transfer. The material achieves remarkable theoretical specific capacities of 2359 mAh g−1 for Li and 1846 mAh g−1 for K, surpassing several advanced 2D materials. Despite substantial volume expansion during metal loading, C[3]A maintains excellent structural reversibility and thermal stability up to 400 K. Electronic structure analysis reveals a significant reduction in the energy gap—particularly in the periodic framework at high metal loading—indicating enhanced electrical conductivity. These outstanding properties, combined with the material's ability to accommodate both Li and K ions efficiently, position C[3]A as a promising candidate for high-performance energy storage applications.