

Electronic Supplementary Information

Coronene: A High-Voltage Anion Insertion and De-Insertion Cathode for Potassium-Ion Battery

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Experimental Section

Materials

Coronene (Sigma-Aldrich; Purity of > 97%) was used as-purchased. Particle morphology was analysed by a field emission scanning electron microscope (JSM-7900F).

Electrochemistry

All electrochemical measurements were performed in K half-cells at room temperature. Assembly of coin cells were conducted in an Ar-purged glove box (MIWA, MDB-1KP-0 type) with O₂ and H₂O contents maintained below 1 ppm. Electrode fabrication protocols were performed in a dry room. Coronene was mixed with polyvinylidene fluoride (PVdF) and carbon black in a weight ratio of active material : binder : carbon in the cathode of 8: 1: 1. A viscous slurry was obtained via suspension in *N*-methyl-2-pyrrolidinone (NMP), which was then cast on aluminium foil with a mass loading of ~4 mg cm⁻². Electrodes were punched and dried at 120 °C in a vacuum oven. In addition, composite electrodes comprising polytetrafluoroethylene were also assembled for a comparison of the electrochemical performance with the composite electrodes fabricated using PVdF. 2032-type coin cells were used to assess the electrochemical properties of coronene. The assembled half-cells comprised coronene (as the composite cathode (positive electrode)) alongside the K metal negative electrode (technically as counter electrode), separated by glass fibre discs soaked with electrolyte. The electrolyte used was a 1 mol dm⁻³ potassium bis(fluorosulphonyl)imide (KFSI) (TCI (Japan, >95.0%) in 1-methyl-1-propylpyrrolidinium bis(fluorosulphonyl)imide (Pyr₁₃FSI) (<20 ppm H₂O, Kanto Chemicals (Japan), 99.9%) ionic liquid. Galvanostatic (dis)charge measurements were performed at various current rates corresponding to C/20 (20 being the necessary hours to (de)insert 1 FSI per formula unit of coronene), C/10, C/5/ C/2, 1C and 2C. For clarity, 1C corresponds to a current density of 88 mA g⁻¹. Cyclic voltammetry tests were conducted between 2.8 V and 4.3 V (vs. K⁺ / K) at a scan rate of 0.1 mV s⁻¹. We detail the electrochemical performance of the composite electrodes composed of PVdF, owing to their superior capacity performance. No electrochemical activity could be discerned at lower voltage regimes (see **Figure S1**).

Electrochemical performances for other polycyclic aromatic hydrocarbons (pentacene, benz[a]anthracene, perylene, chrysene, naphthalene and triphenylene) were evaluated using stable electrolytes based on bis(trifluoromethanesulphonyl)imide ionic liquids. Although no electrochemical activity was found in chrysene, naphthalene and triphenylene, relatively high voltages were attained in perylene, benz[a]anthracene and pentacene (as shown in **Figure S2**).

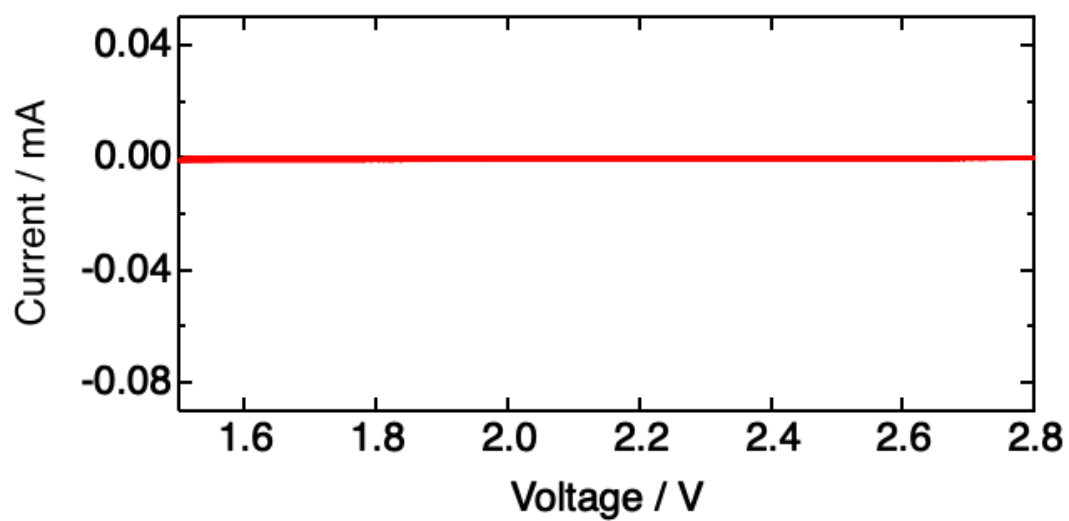


Figure S1. Cyclic voltammograms of coronene taken at a voltage range of 1.5–2.8 V and at a scanning rate of 0.1 mV s^{-1} . No peaks were observed during both the cathodic and anodic scans. This indicates that there is no redox activity associated with cation insertion into coronene. Therefore, it is not possible to use coronene as an *n*-type cathode material.

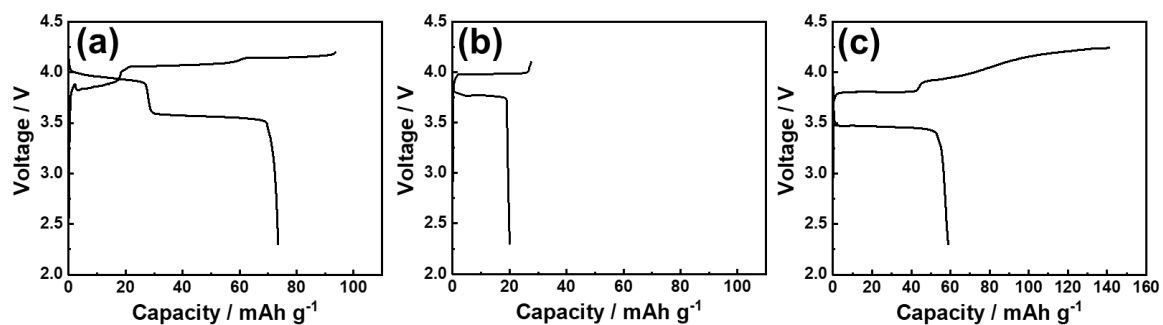


Figure S2. Voltage-capacity plots for (a) perylene, (b) benz[a]anthracene and (c) pentacene in potassium half-cells. The electrolyte used was a 0.5 mol dm⁻³ potassium bis(trifluoromethanesulphonyl)imide (KTFSI) in 1-methyl-1-propylpyrrolidinium bis(trifluoromethanesulphonyl)imide (Pyr₁₃TFSI) ionic liquid. The cut-off voltage was set at 4.2 V – 2.3 V.