
Supporting Information

Iridium-decorated carbon nanotubes as cathode catalysts for Li-CO₂ batteries with a highly efficient direct Li₂CO₃ formation/decomposition capability

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Keywords: Li-CO₂ Batteries, Electrocatalysis, Cathode Catalyst, Ir-CNTs Composite, DFT Calculations

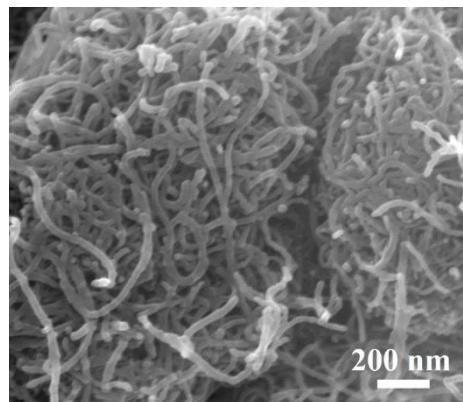


Figure S1. SEM image of the Ir-CNT composite.

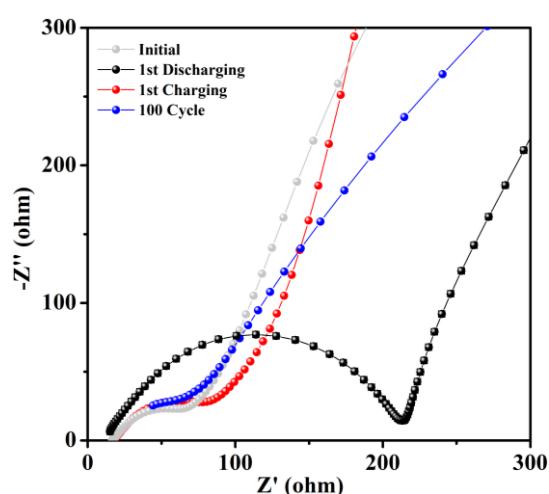


Figure S2. Electrochemical Impedance Spectroscopy (EIS) dates at different stages of Ir-CNT cathodes.

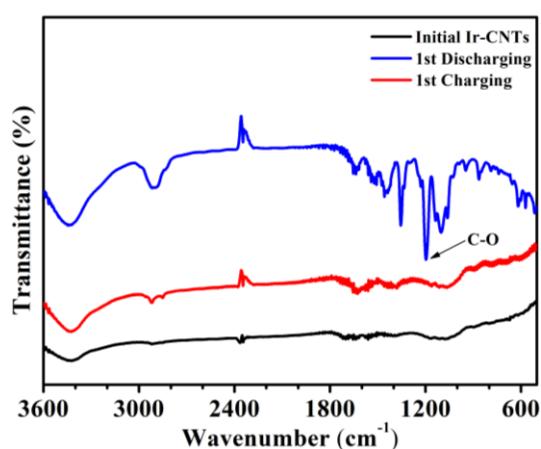


Figure S3. FTIR spectra of Ir-CNT cathodes at initial, 1st discharging and 1st charging stage.

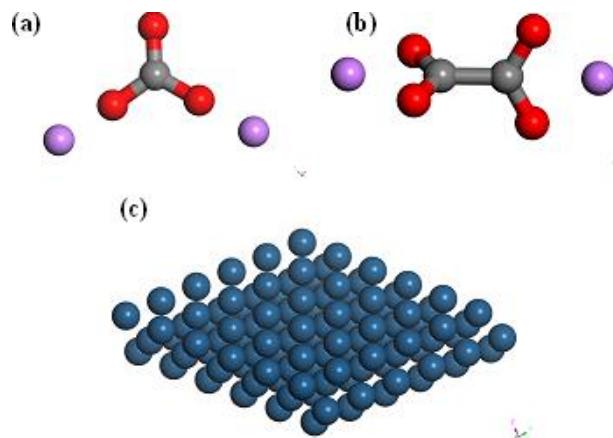


Figure S4. Schematic illustrations of (a) Li_2CO_3 monomer, (b) Li_2CO_4 monomer and (c) Ir (111) models.

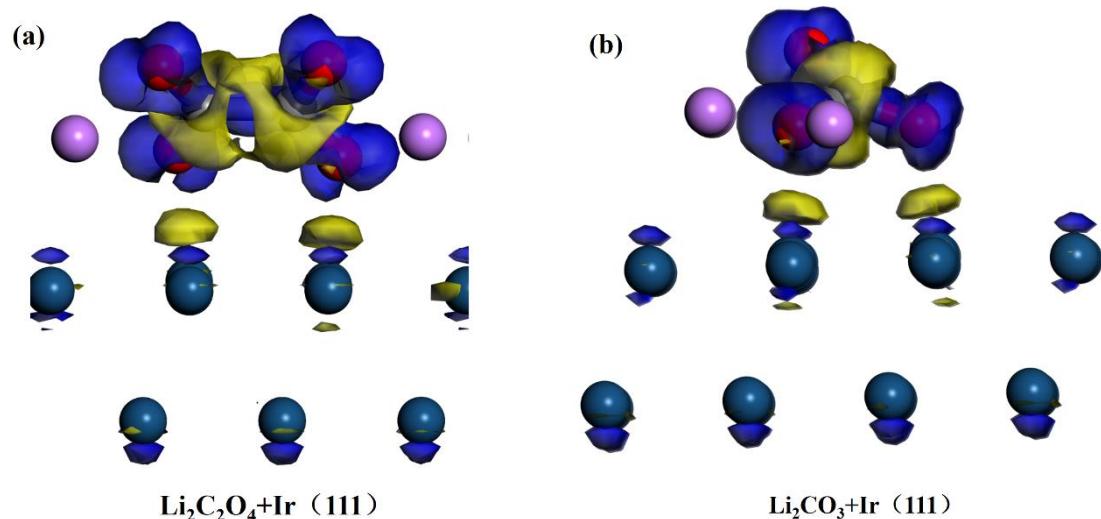


Figure S5. Difference charge densities and corresponding binding models of (a) $\text{Li}_2\text{C}_2\text{O}_4$ monomer on Ir (111) plane and (b) Li_2CO_3 monomer on Ir (111) plane.

Table 1. Performance comparison of the Ir-CNT cathode with other typical cathodes reported in the literature.

Catalyst	Discharge product	Main Electrolyte	Current Density (mA g^{-1})/ Fixed Capacity (mAh g^{-1})/ Cycles	Ref. No
Ir-coated GDLs	Li_2CO_3	DOL	100/500/150	1
Li_2MnO_3	Li_2CO_3	DMC	/800/30	2
CNTs	Li_2CO_3	polymer	500/1000/20	3
CPE@CNTs	Li_2CO_3	polymer	2.5 mA/993.3 mAh/44	4
CC@Mo_2C	$\text{Li}_2\text{C}_2\text{O}_4$	TEGDME	50 $\mu\text{A cm}^{-2}$ /100 $\mu\text{Ah cm}^{-2}$ /20	5
$\text{Mo}_2\text{C/CNT}$	$\text{Li}_2\text{C}_2\text{O}_4$	TEGDME	20 $\mu\text{A}/100 \mu\text{Ah}/40$	6
Ru/NS-G	Li_2CO_3	TEGDME	100/1000/100	7
MnO@NC-G	Li_2CO_3	TEGDME	50/1000/15	8
CoPPc	Li_2CO_3	TEGDME	0.05 mA cm^{-2} //50	9
Adj. Co/GO	Li_2CO_3	TEGDME	100/1000/100	10
Ir/CNFs	Li_2CO_3	TEGDME	50/1000/45	11
Ir-CNTs	Li_2CO_3	TEGDME	100/1000/100	This Work

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