

Single-Walled Carbon Nanotubes with Red Phosphorus in Lithium-Ion Batteries: Effect of Surface and Encapsulated Phosphorus

Anna A. Vorfolomeeva¹, Svetlana G. Stolyarova¹, Igor P. Asanov¹, Elena V. Shlyakhova¹, Pavel E. Plyusnin¹, Evgeny A. Maksimovskiy¹, Evgeny Yu. Gerasimov², Andrey L. Chuvilin^{3,4}, Alexander V. Okotrub¹ and Lyubov G. Bulusheva^{1,*}

¹ Nikolaev Institute of Inorganic Chemistry SB RAS, 3 Acad. Lavrentiev Ave., 630090 Novosibirsk, Russia

² Boreskov Institute of Catalysis, SB RAS, 5 Acad. Lavrentiev Ave., 630090 Novosibirsk, Russia

³ CIC NanoGUNE BRTA, Tolosa Hiribidea 76, E-20018 Donostia-San Sebastián, Spain

⁴ IKERBASQUE, Basque Foundation of Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain

* Correspondence: bul@niic.nsc.ru; Tel.: +73-8333-053-52

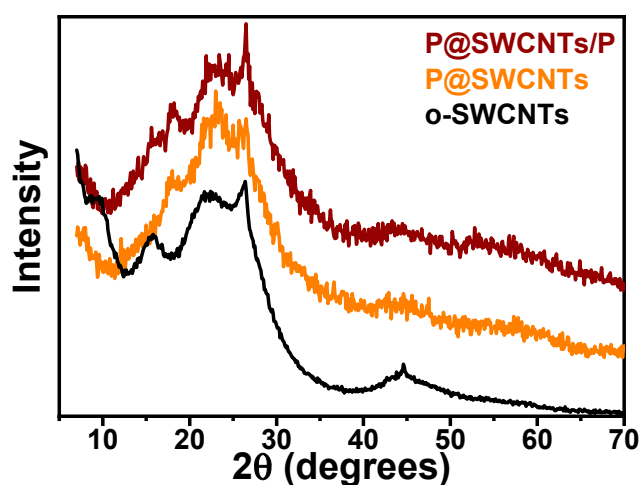


Figure S1. XRD patterns measured for initial o-SWCNTs and P@SWCNTs/P, P@SWCNTs samples.

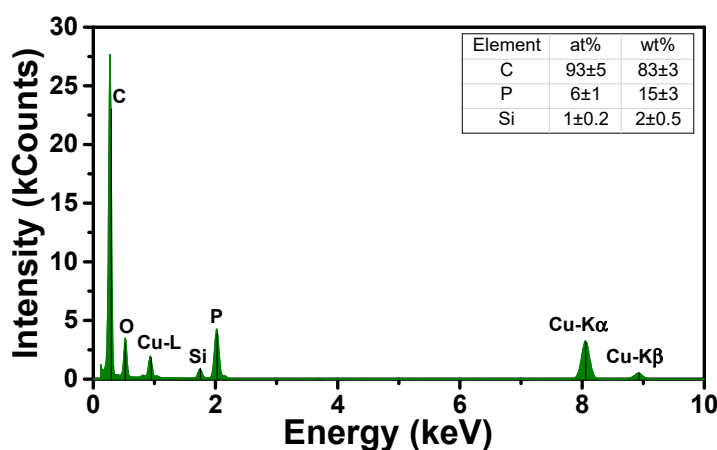


Figure S2. EDS analysis of P@SWCNTs sample. The spectrum and content of the main elements (inserted table). Cu and O are associated with the TEM grid, Si is impurity from the quartz ampoule.

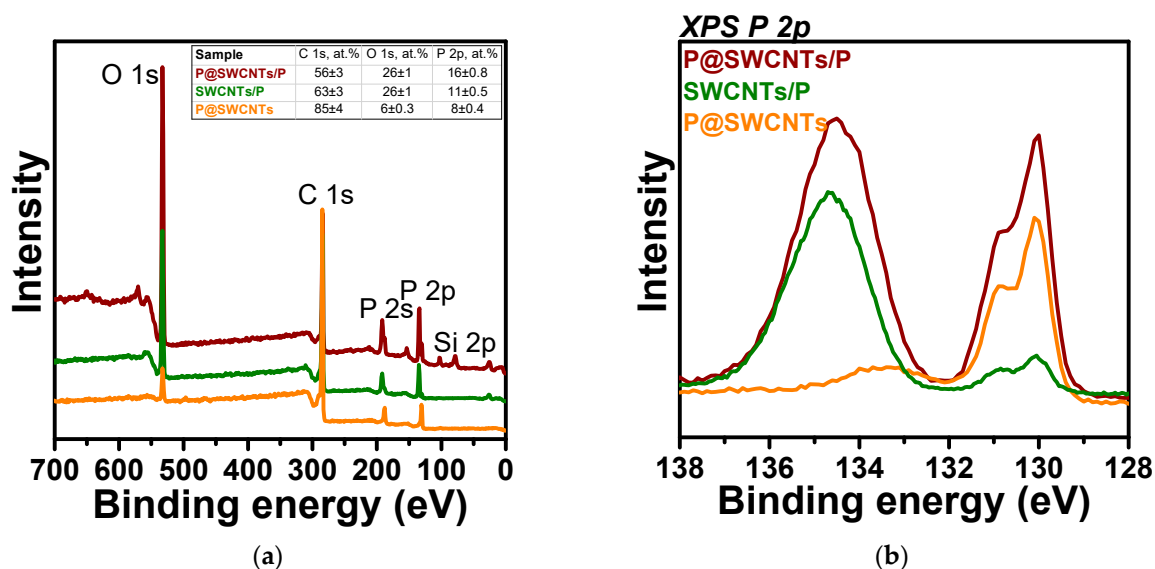


Figure S3. (a) Survey XPS spectra and (b) XPS P 2p spectra of P@SWCNTs (encapsulated phosphorus), SWCNTs/P (external phosphorus), and P@SWCNTs/P (encapsulated and external phosphorus). Inset shows the concentrations of carbon, oxygen, and phosphorus in the samples.

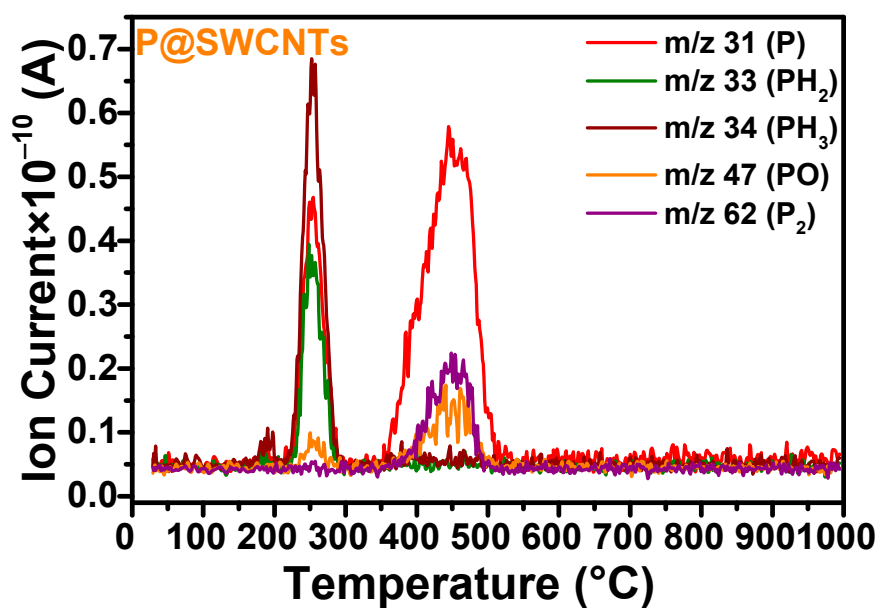


Figure S4. Ion current curves of evolved gases during decomposition of P@SWCNTs sample.

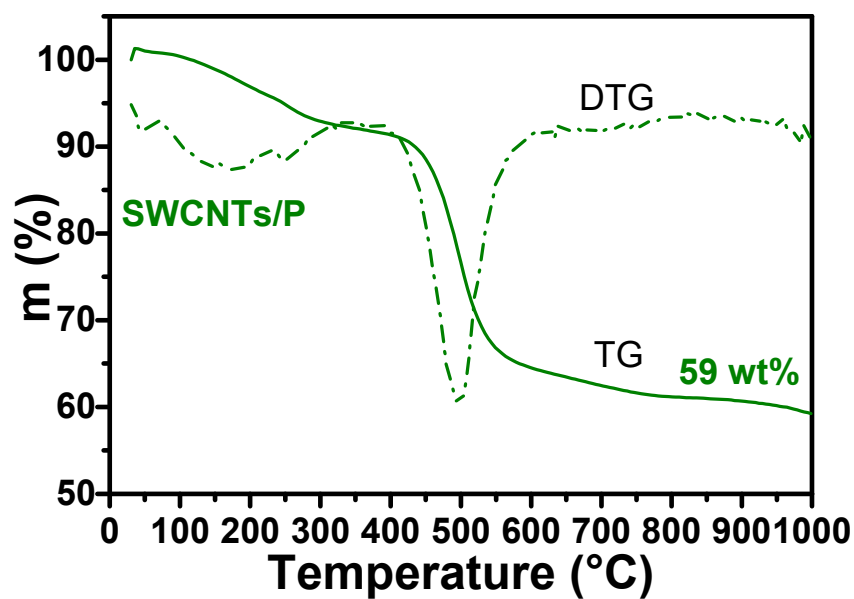


Figure S5. TG and DTG curves measured for SWCNTs/P in helium.

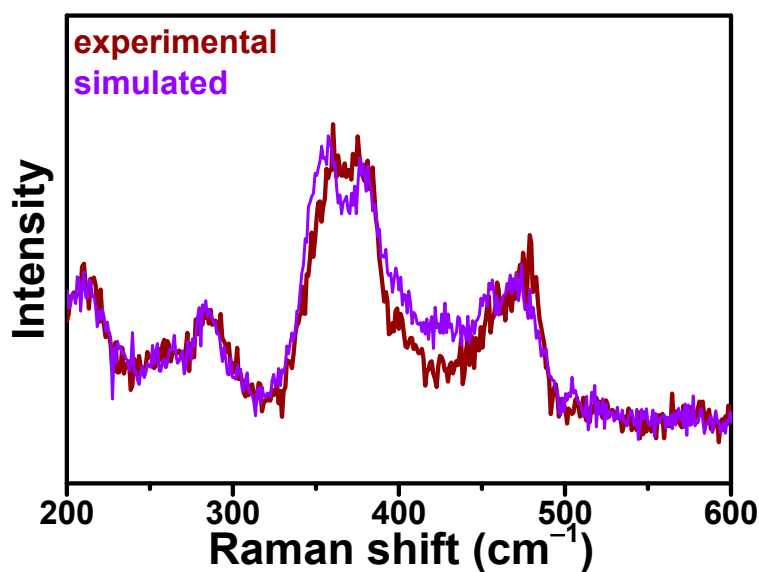


Figure S6. Experimental Raman spectrum of P@SWCNTs/P and the spectrum simulated using the spectra of recrystallized phosphorus P_{re} and P@SWCNTs in a ratio of 0.3 to 1.1.

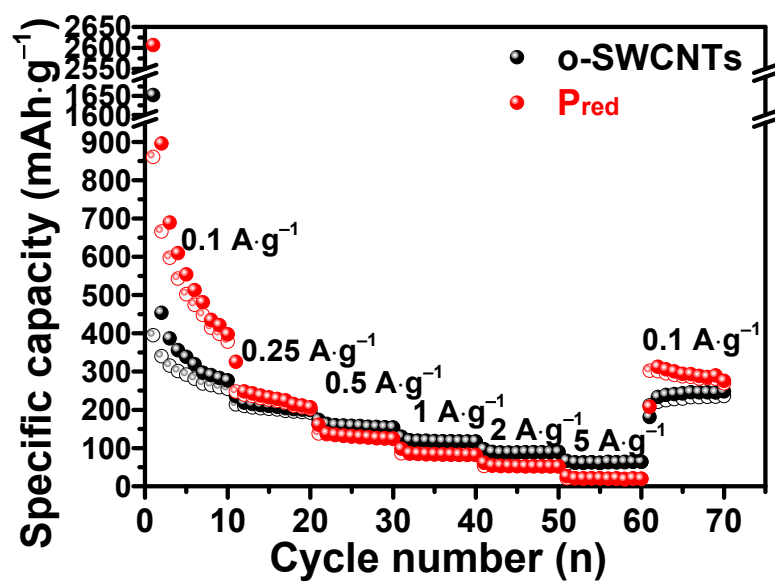


Figure S7. Rate performance of o-SWCNTs and commercial red phosphorus (P_{red}).

Table S1. Electrochemical performance of P–CNT composites in lithium-ion batteries.

Sample	Synthesis	P content	Current density, A g ⁻¹	Specific capacity (mAh g ⁻¹) of carbon	Specific capacity (mAh g ⁻¹) based on the composite mass	Specific capacity (mAh g ⁻¹) based on the phosphorus mass	Cycle performance	Reference
P-SCNT	vaporization-condensation (vacuum, 700 °C, 4 h)	36 wt%	0.1	~400	1398	–	1400 mAh g ⁻¹ at 100 mA g ⁻¹ after 200 cycles	29
			2		782	–		
P-CNT	ball-milling (Ar, 500 rpm, 40 h)	?	0.78	~70	–	1771	1844 mAh g ⁻¹ at 780 mA g ⁻¹ after 300 cycles	17
			3.90		–	1081		
ARPC-48	ball-milling (Ar, 450 rpm, 48 h)	?	0.016 (0.01 C)	?	1994 (не указано)		999 mAh g ⁻¹ at 0.05 C after 50 cycles	2
			0.8 (0.5 C)	?	817			
P@CNT	solution-based method, ultrasonicated 5 min at room temperature	72 wt%	0.2	235–178	1082	1997–1264	736 mAh g ⁻¹ at 1000 mA g ⁻¹ after 450 cycles	79
			10	–	784	–		
P@DMWCNTs	gas-phase synthesis (vacuum, 550 °C, 10 h)	58 wt%	0.025	~350	~500	834	834 mAh g ⁻¹ at 25 mA g ⁻¹ after 50 cycles	41
PP@MWCNTs	solution-based method (Ar, 189 °C, 8 h)	32 wt%	0.1	?	–	886	886 mAh g ⁻¹ at 100 mA g ⁻¹ after 500 cycles	39
			3	?	–	~400		
r-P@MWCNTs	vaporization-condensation (vacuum, 500 °C, 48 h, gradient cooling)	16 wt%	0.1	~500	446	–	444 mAh g ⁻¹ at 500 mA g ⁻¹ after 500 cycles	44
			3	~300	246	–		
RP-on-r-P@MWCNTs	vaporization-condensation (vacuum, 500 °C, 48 h, natural cooling)	72 wt%	0.1	~500	780	–	<444 mAh g ⁻¹ at 500 mA g ⁻¹ after 500 cycles	44
			3	~300	~700	–		
P-MWCNTs	wet ball-milling (Ar, 650 rpm, 7 h)	?	0.05	143	1615	–	1397 mAh g ⁻¹ at 50 mA g ⁻¹ after 50 cycles	20
			1	–	934	–		
RP NPs/MWNT	solution-based method (100 °C, 2 h)	56 wt%	0.2	?	1612	–	1577 mAh g ⁻¹ at 200 mA g ⁻¹ after 100 cycle	80
			3	?	~1200	–		
P–SWCNT	hand-grinding; vaporization-condensation at 600 °C, 2 h	60 wt%	0.05	~130 at 150 mA/g	434	–	398 mAh g ⁻¹ at 150 mA g ⁻¹ after 100 cycles	40
			1	–	160	–		
SWCNT/P	Hand-grinding, vaporization-condensation at 600 °C, 2h	70 wt%	0.05	–	800	–	~350 mAh g ⁻¹ at 50 mA g ⁻¹ on 80 th cycle	81
P@SWCNTs	vaporization-condensation (vacuum, 800 °C, 48 h, natural cooling)	28 wt%	0.1 A/g	245	609	1545	317 mAh g ⁻¹ at 5000 mA g ⁻¹ after 1000 cycles	This work
			5 A/g	61	328	1006		
P@SWCNTs/P		51 wt%	0.1 A/g	245	578	900	248 mAh g ⁻¹ at 5000 mA g ⁻¹ after 1000 cycles	
			5 A/g	61	279	486		