## Supporting Information

## Coronene based Graphene Nanoribbons Insulated by Boron Nitride Nanotubes; towards Electronic Properties of the Hybrid Structure

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**Figure S1**. Coronene-based 7-GNR. (a) The super cell consist of two coronene molecules with a lattice parameter along the growth direction of 17.29 Å. (b) Density of States (DOS) of the 7-GNR at the equilibrium lattice parameter (17.29 Å) and at expanded lattice of 17.56 Å. (c) Defective 12-GNR. (d) DOS at the equilibrium lattice parameter of 17.39 and at the expanded lattice of 17.56 Å.



**Figure S2.** Optimized geometry of (a) pristine and (b) defective 12-GNR encapsulated inside a (16,16)-BNNT. The lattice parameter is 17.56 Å for both systems.



**Figure S3.** Optimized structure of (a) 4-zigzag (4-zGNR) and (b) 7-armchair (7-aGNR) graphene nanoribbons inside a (12,12)-BNNT. (c-d) Density of states of the isolated and composite systems.



**Figure S4.** Optimized geometries of non-defective 12-GNR at different twisting rates. The distance indicates the necessary length to achieve a half-turn, and the units specify the number of unit cells in each system. Similar configurations are observed for the 7-GNRs as well as the defective systems.

-			10 0 0	/
	Eg = ´	1.41 eV	(†) 0.5	o0π/unit
Mm M	A		$\mathbb{A}$	h
	Eg =	1.15 eV	(e) 0.3	33π/unit
hml	A	∟~∿	h	-1
	Eg =	1.04 eV	(d) 0.2	25π/unit
hond	A	^	h	_1
	Eg = (	0.95 eV	(c) 0.1	6π/unit
mm	Λ		h	
m	<u>∧</u> Eg = 0	0.91 eV	(b) 0.	 I2π/unit
mp.M.	<u>∧</u> Eg = 0	0.91 eV	(b) 0 	$12\pi/unit$
mp.M.	Eg = 1 Eg = 1 <u>A</u> Eg =	0.91 eV	(b) 0 (b) 0 (a) 0.(	$12\pi/\text{unit}$ $12\pi/\text{unit}$ $12\pi/\text{unit}$
mp.M. mp.M. hM.M.	Eg = 1 Eg = 1 Eg =	0.91 eV	(b) 0.7	$12\pi/unit$ $12\pi/unit$ $00\pi/unit$
-4 -2	Eg = ( Eg = ( Eg = (	0.91 eV 0.92 eV	(b) 0.7 (a) 0.0 (a) 0.0 2	$\frac{12\pi/\text{unit}}{12\pi/\text{unit}}$

Figure S5. DOS of 7-GNR at different twisting rates.

	Eg = 1	.18 eV	(f) 0.50π/	/unit
homen	M	M	M	M
	Eg = 1	.36 eV	(e) 0.33π	/unit
Mohn	M	h nam	Mm	<u>`</u> ~^
	Eg = 1	.39 eV	(d) 0.25π	/unit
Mmm	M	~ M	M	
	Eg = 1	.32 eV	(c) 0.16π/	unit
An			٨	
	<u>M</u>	$i \sim M$	<u>M</u>	_^
	<u></u> Eg = '	1.36 eV	(b) 0.12π/	/unit
Mann	<u></u> Eg = ` <u></u>	1.36 eV	(b) 0.12π/	 /unit 
MM	<u></u> Eg = ^ <u></u> Eg = 1	1.36 eV .52 eV	(b) 0.12π/ (a) 0.00π/	/unit /unit /unit
Mann-	<u></u> Eg = <sup>-</sup> <u>M</u> Eg = 1 <u>M</u>	.36 eV .52 eV	(b) 0.12π/ (a) 0.00π/	/unit /unit /unit
$M_{m}$	$\frac{M}{Eg} = \frac{1}{2}$ $\frac{M}{Eg} = 1$ $\frac{M}{M}$ (	.36 eV .52 eV	(b) 0.12π/ (a) 0.00π/ 2	 /unit /unit

Figure S6. DOS of defective 7-GNR at different twisting rates.



Figure S7. DOS of (a) non-defective and (b) defective 12-GNRs at different twisting rates.



**Figure S8.** Optimized geometries of (a) non-defective and (b) defective 7-GNR@(12,12)-BNNT twisted at  $0.50\pi$  rad/unit, and their respective (c) density of states. The lattice parameter for both systems is 17.56 Å. Optimized geometries of (d) non-defective and (e) defective 12-GNR@(16,16)-BNNT twisted at  $0.25\pi$  rad/unit with their respective (f) density of states. The lattice parameter for both systems is 35.12 Å.



**Figure S9.** Device configuration used to calculate the electron transport properties for (a) Planar 7-GNR, (b) twisted 7-GNR, (c) planar 12-GNRs and (d) twisted 12-GNR. Similar device configurations are used for defective 7- and 12-GNRs.