

## Supporting Information

# Synergistic ZnS/MWCNT Heterostructure as Advanced Electrode for High-Performance, Long-Cyclic Lithium-Ion Batteries: Experimental and DFT Insights

Marrium Shabbir <sup>a, b</sup>, Rizwan Akram <sup>b</sup>, Saqib Javed <sup>c</sup>, Zahid Abbas <sup>a, d</sup>, Amina Zafar <sup>e</sup>, Sheeraz Mehboob <sup>f</sup>, Shafqat Karim <sup>a</sup>, Luqman Ali <sup>a, g</sup>, Shahid Ali <sup>a, d</sup>, Imran Shakir <sup>h</sup>, Amjad Nisar<sup>\*a</sup> and Mashkoor Ahmad<sup>\*a</sup>

*a Nanomaterials Research Group, Physics Division, PINSTECH, Islamabad 44000, Pakistan.*

*b Department of Applied Physics, Air University, Islamabad, Pakistan.*

*c Theoretical Physics Division, PINSTECH, Islamabad 44000, Pakistan*

*d Department of Chemistry Govt. College University, Faisalabad.*

*e Central Analytical Facility Division, PINSTECH, Islamabad 44000, Pakistan*

*f Physics Division, PINSTECH, Islamabad 44000, Pakistan.*

*g Department of Chemistry, University of Poonch, Rawalakot.*

*h Department of Physics, Faculty of Science, Islamic University of Madinah, Madinah 42351, Saudi Arabia.*

*Electronic Supplementary Information (ESI) available See DOI: 10.1039/x0xx00000x*

Correspondence:

[mashkoorahmad2003@yahoo.com](mailto:mashkoorahmad2003@yahoo.com) (Mashkoor Ahmad)

[chempk@gmail.com](mailto:chempk@gmail.com) (Amjad Nisar)

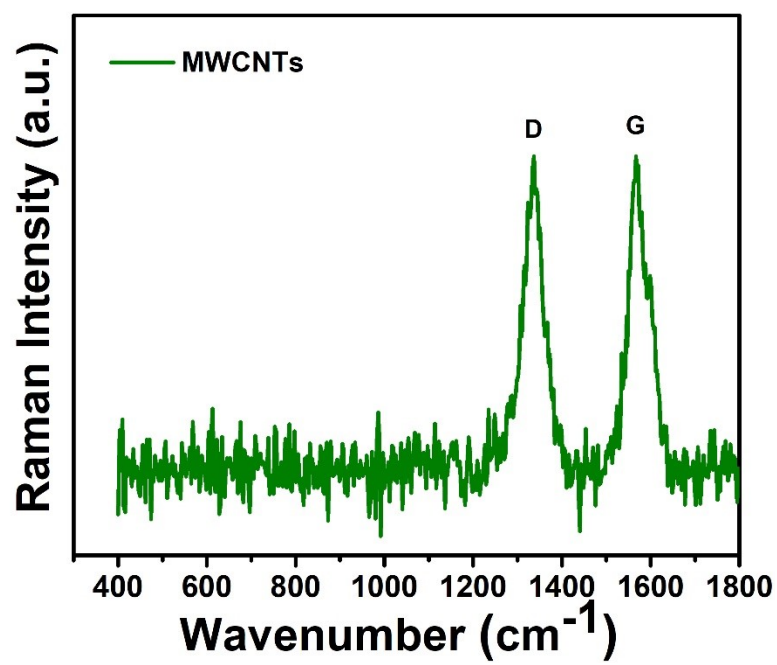
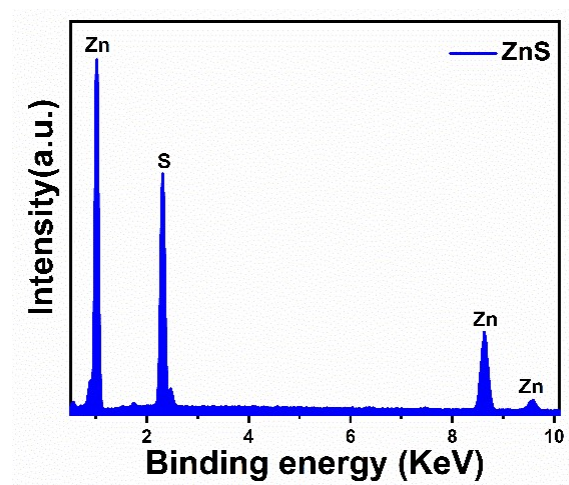
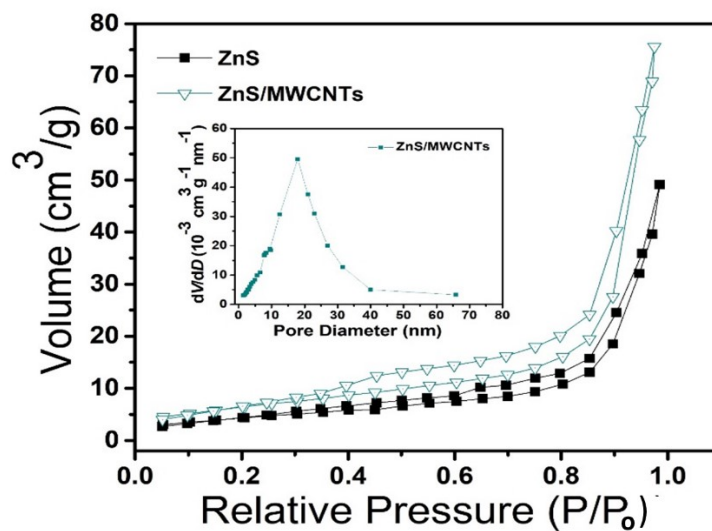


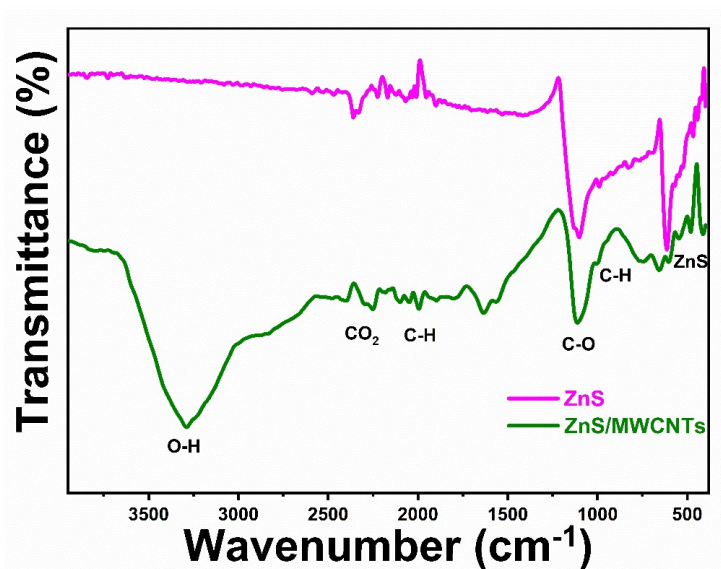
Figure S1. Raman spectrum of pure MWCNTs.



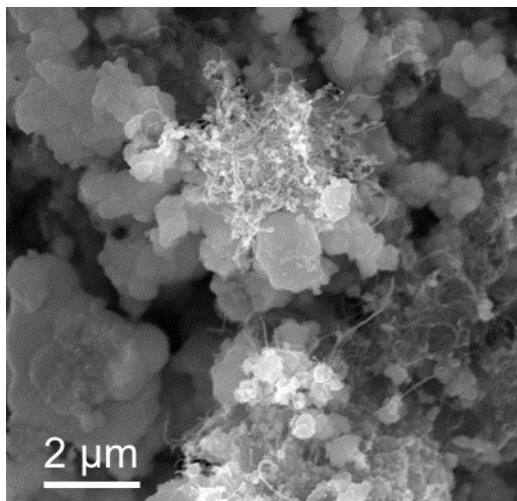
**Figure S2.** EDX Spectra of pristine ZnS



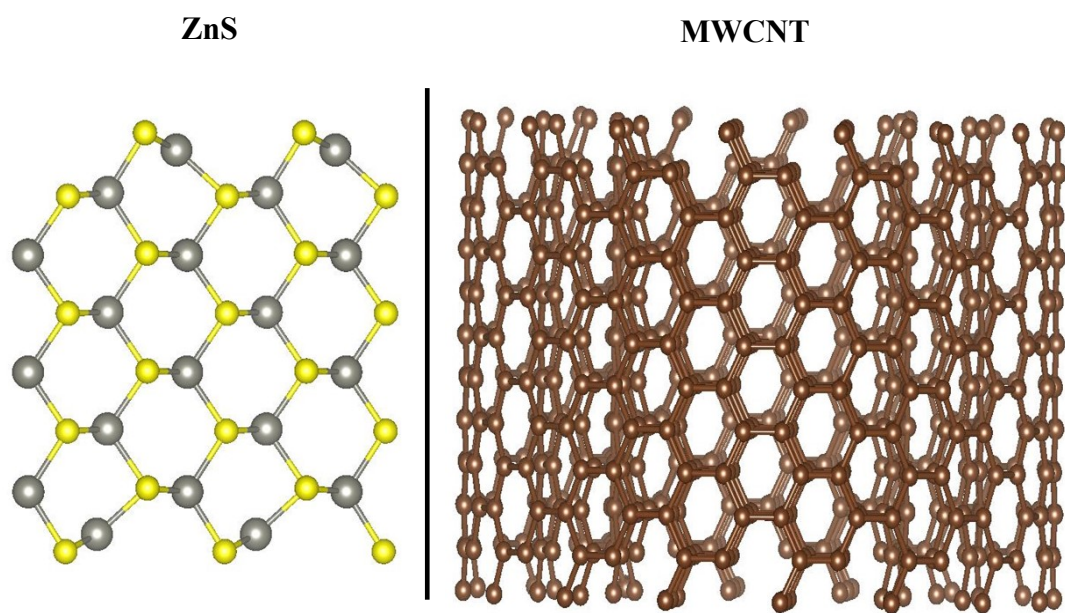
**Figure S3.** BET specific surface area of ZnS and ZnS/MWCNTs; Inset is the pore size distribution of ZnS/MWCNTs heterostructure.



**Figure S4.** FTIR spectrum of pristine ZnS and heterostructured ZnS/MWCNTs



**Figure S5.** SEM of the ZnS/MWCNT structure after 1000 charge–discharge cycles.



**Fig.S6:** A schematic depiction of heterostructure between MWCNT and ZnS (110) surface.