

ARTICLE

Hydrothermal Synthesized 2H-WS₂ Nanorods for Improved Supercapacitor Electrode Performance

Received 00th January 20xx,
Accepted 00th January 20xx

Somveer,^a Rohit Yadav,^b Jitesh Pani,^b Rakesh Nanna,^b Ranjit Kumar,^{c,d} Vinay S. Palaparthi,^e Kusum Kumari,^b Davender Singh,^f Dharamvir Singh Ahlawat,^{*a} Hitesh Borkar^{*b} and Jitendra Gangwar^{*f}

DOI: 10.1039/x0xx00000x

Table S1 provides the calculated distinctive electronic properties including dipole moment, E_{HOMO} , E_{LUMO} , electron affinity, ionization potential, chemical potential, electronegativity, chemical hardness, charge transfer and nucleophilic index for WS₂ structure and WS₂ attached with K⁺.

Table S1 Calculated electronic properties of WS₂ and WS₂ with K⁺.

Electronic Properties	WS ₂	WS ₂ with K
Dipole moment	4.269×10^{-32} Cm	2.129×10^{-29} Cm
E_{HOMO}	- 5.731 eV	- 3.117 eV
E_{LUMO}	- 4.578 eV	- 2.449 eV
$E_{\text{LUMO}} - E_{\text{HOMO}}$ (ΔE)	1.153 eV	0.668 eV
Electron affinity (EA) = $-E_{\text{LUMO}}$	4.578 eV	2.449 eV
Ionisation potential (IP) = $-E_{\text{HOMO}}$	5.731 eV	3.117 eV
Chemical potential (χ) = $-(E_{\text{LUMO}} + E_{\text{HOMO}})/2$	- 5.155 eV	-2.783 eV
Electronegativity (μ) = $-(E_{\text{LUMO}} + E_{\text{HOMO}})/2$	5.155 eV	2.783 eV
Chemical hardness (η) = $(E_{\text{LUMO}} - E_{\text{HOMO}})/2$	0.577 eV	0.334 eV
Charge transfer (ΔN_{max}) = $-(\mu/\eta)$	- 8.934	- 8.332
Nucleophilic index (ω) = $-(\mu^2/2\eta)$	- 23.027	- 11.593

Fig. S1 demonstrates the comparative CV curves for different electrolytes at scan rate of 100 mV/s.

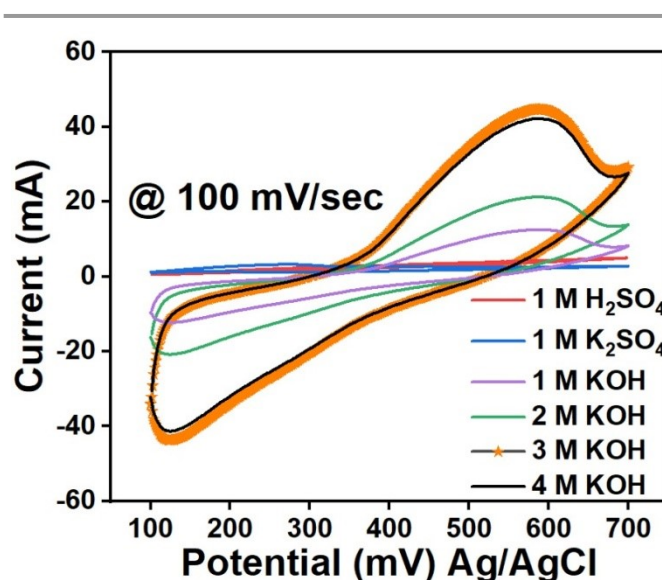


Fig. S1 Comparative CV curves stating at different electrolyte at 100 mV/Sec scan rate.

^a Department of Physics, Chaudhary Devi Lal University, Sirsa, Haryana 125055, India.

^b Department of Physics, National Institute of Technology, Warangal, Telangana, 506004, India.

^c Department of Physics, Arignar Anna Government Arts and Science College, Karaikal, UT of Puducherry 609605, India.

^d Department of Physics, Dr. Kalaignar M. Karunanidhi Government Institute for Postgraduate Studies and Research, Karaikal, UT of Puducherry 609605, India.

^e System Design Laboratory, Information and Communication Technology, Dhirubhai Ambani Institute of Information and Communication Technology, Gujarat 382007, India.

^f Department of Physics, RPS Degree College, Balana, Mahendergarh, Haryana 123029, India.

Supplementary Information available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x