

## SUPPLEMENTARY MATERIAL

### Role of defect engineering in revealing electronic and sensing applications of Janus WSSe monolayer

Bindiya Babariya<sup>a</sup>, Sanjeev K. Gupta<sup>b,\*</sup> and P. N. Gajjar<sup>a,\*</sup>

<sup>a</sup>Department of Physics, University School of Sciences, Gujarat University, Ahmedabad 380009, India.

<sup>b</sup>Computational Materials and Nanoscience Group, Department of Physics and Electronics, St. Xavier's College, Ahmedabad 380009, India.

**Keyword (s):** Janus MoSSe monolayer, Pd/Pt adatom decoration, CH<sub>4</sub> sensing, DFT

\*Corresponding authors: Prof. (Dr.) P. N. Gajjar (E-mail: pngajjar@gujaratuniversity.ac.in, pngajjar@rediffmail.com) and Dr. Sanjeev K. Gupta (E-mail: sanjeev.gupta@sxca.edu.in)

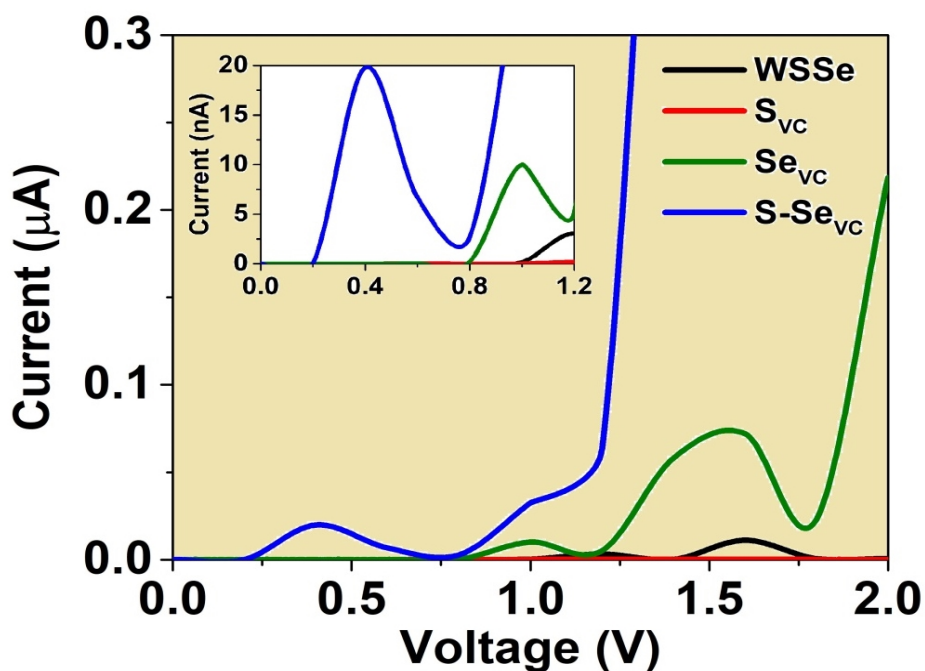


Figure S1 I-V characteristics of pristine and defected MoSSe monolayer before adsorption

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Table S1 The calculated PVCR at particular voltage with NDR existence

System	Gas molecules	Voltage (V)	PVCR
WSSe_S	CH <sub>4</sub>	0.8	12.8
		1.4	5.71
	C <sub>3</sub> H <sub>8</sub>	1.4	13.7
		0.6	29.5
WSSe_Se	CH <sub>4</sub>	1.2	5.78
		0.4	1.72
	C <sub>3</sub> H <sub>8</sub>	1.4	7.16
		0.8	4.80
S <sub>vc</sub>	C <sub>4</sub> H <sub>10</sub>	1.0	6.55
		0.6	12.0
	CH <sub>4</sub>	1.2	13.9
		0.8	3.67
Se <sub>vc</sub>	C <sub>4</sub> H <sub>10</sub>	0.4	15.0
		1.6	5.66
	CH <sub>4</sub>	1.6	5.07
		0.8	6.28
S-Se <sub>vc</sub> _S	C <sub>4</sub> H <sub>10</sub>	1.4	8.19
		1.6	1.25
	C <sub>3</sub> H <sub>8</sub>	0.4	9.28
		1.6	1.36
S-Se <sub>vc</sub> _Se	C <sub>4</sub> H <sub>10</sub>	0.2	2.97
		1.4	1.31
	CH <sub>4</sub>	1.4	1.07
		1.2	1.70
	C <sub>4</sub> H <sub>10</sub>	1.6	1.77

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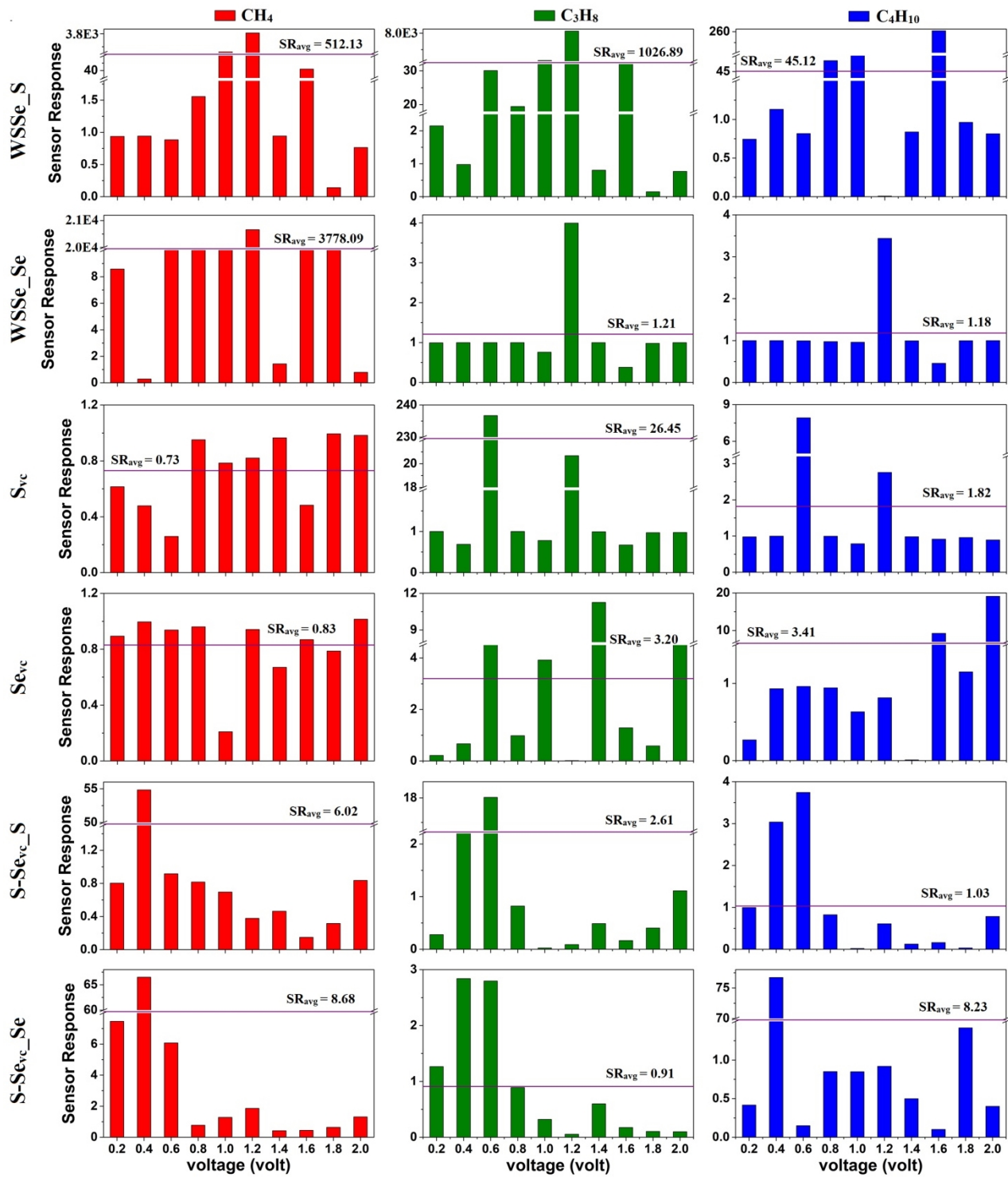


Figure S2 Sensor response at particular bias voltage for pristine and defected WSe monolayer after gas adsorption

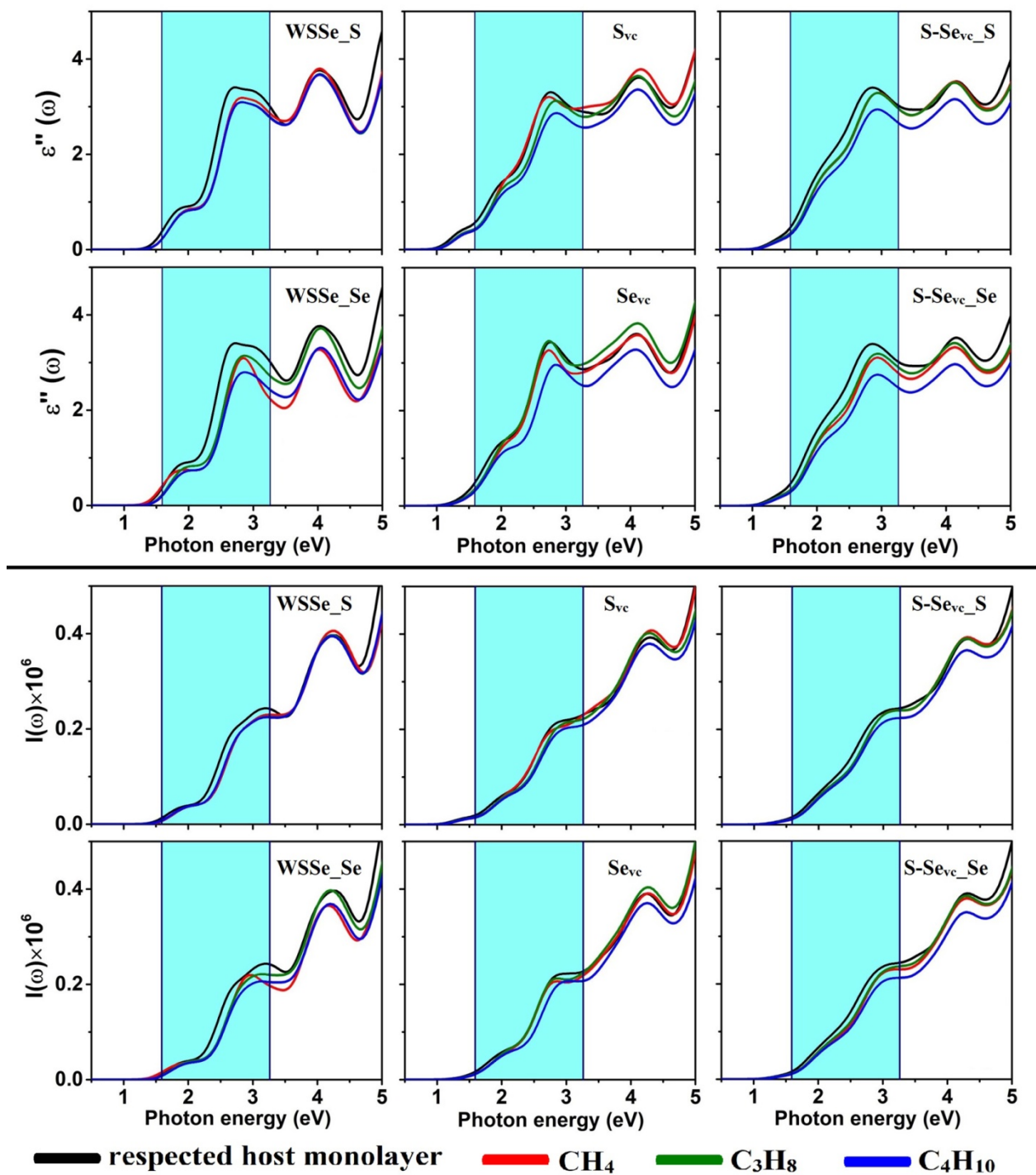


Figure S3 Imaginary part of dielectric function and absorption spectra along the directions of parallel to the optical vector axis.