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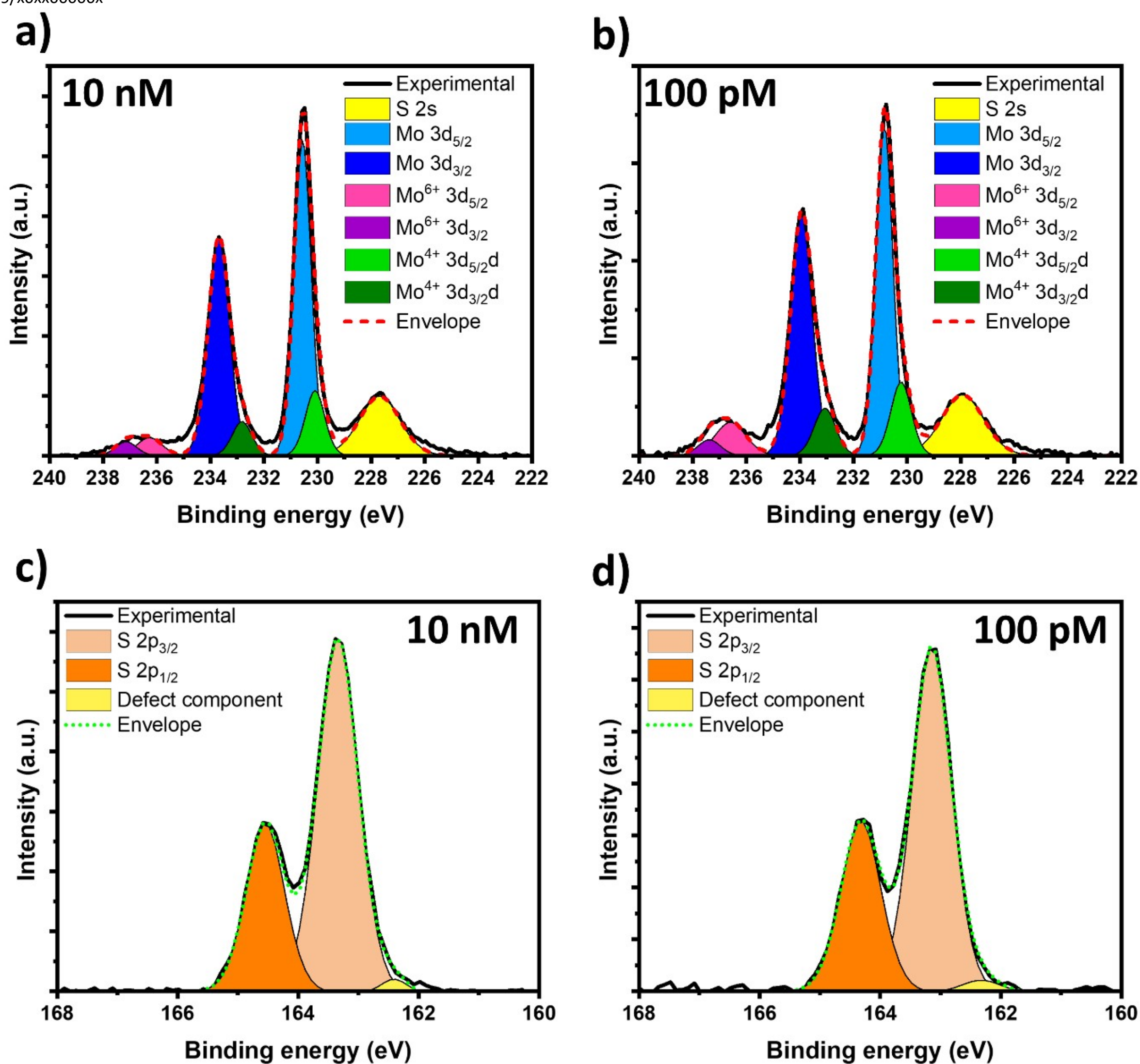
Electronic Supplementary Information

Field-Effect Transistors Based Ion Sensors: Ultrasensitive Mercury (II) Detection via Healing of MoS_2 Defects

Fernando J. Urbanos,[a] Sara Gullace[a] and Paolo Samorì *[a]

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

DOI: 10.1039/x0xx00000x



[a] University of Strasbourg CNRS, ISIS UMR 7006. 8 Allée Gaspard Monge, Strasbourg F-67000, France
* E-mail: samori@unistra.fr
Electronic Supplementary Information (ESI) available: See DOI: 10.1039/x0xx00000x

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Fig S1: High-resolution XPS spectra of CVD MoS_2 exposed to different Hg^{2+} concentrations. **a)** and **b)** Mo 3d XPS spectra at 10 nM and 100 pM, respectively. After deconvolution of the peaks, contribution coming from defective Mo^{4+} is decreasing with increasing Hg^{2+} concentration. **c)** and **d)** S 2p XPS spectra at 10 nM and 100 pM, respectively. Again, the defect component's intensity is decreasing with increasing concentration, indicating defect healing.

	Peak Contribution (%)			
	Control	**100 pM**	**10 nM**	**1 µM**
Mo $3d_{5/2}$	30.08	32.26	35.39	35.63
Mo $3d_{3/2}$	29.92	30.00	30.55	32.74
Mo^{6+} $3d_{5/2}$	7.25	6.08	3.12	2.77
Mo^{6+} $3d_{3/2}$	2.85	2.16	2.05	1.63
Mo^{4+} def $3d_{5/2}$	9.38	8.73	8.36	7.63
Mo^{4+} def $3d_{3/2}$	6.38	5.96	4.53	2.63
S 2s	13.88	14.82	15.99	16.97
S $2p_{1/2}$	31.15	31.97	30.45	31.49
S $2p_{3/2}$	62.42	65.99	67.68	67.24
Defects	6.43	2.45	1.67	1.27

Table S1: Peak contribution (in %) of every component after deconvolution of the high-resolution Mo 3d and S 2p XPS spectra as a function of different Hg^{2+} concentrations. Mo^{4+} defective component, associated to sulphur vacancies, and the so called "defects" decreased when increasing the Hg^{2+} concentration, confirming defect healing.

	Peak Contribution (%)											
	Control			**100 pM**			**10 nM**			**1 µM**		
	M1	**M2**	**M3**	**M4**	**M5**	**M6**	**M7**	**M8**	**M9**	**M10**	**M11**	**M12**
S 2p def	6.43	6.99	6.06	2.45	3.48	2.87	1.67	1.76	1.76	1.27	1.56	1.41
Mean	6.49			2.93			1.73			1.41		
SD	0.47			0.52			0.05			0.15		

Table S2: Peak contribution (in %) of the defect related component after deconvolution of the high-resolution S 2p XPS spectra as a function of different Hg^{2+} concentrations on a total of 12 points (M1-M12) on the CVD MoS_2 sample. Mean and standard deviation (SD) values have been calculated, proving that the defectiveness of the sample decreases by increasing the Hg^{2+} concentration.

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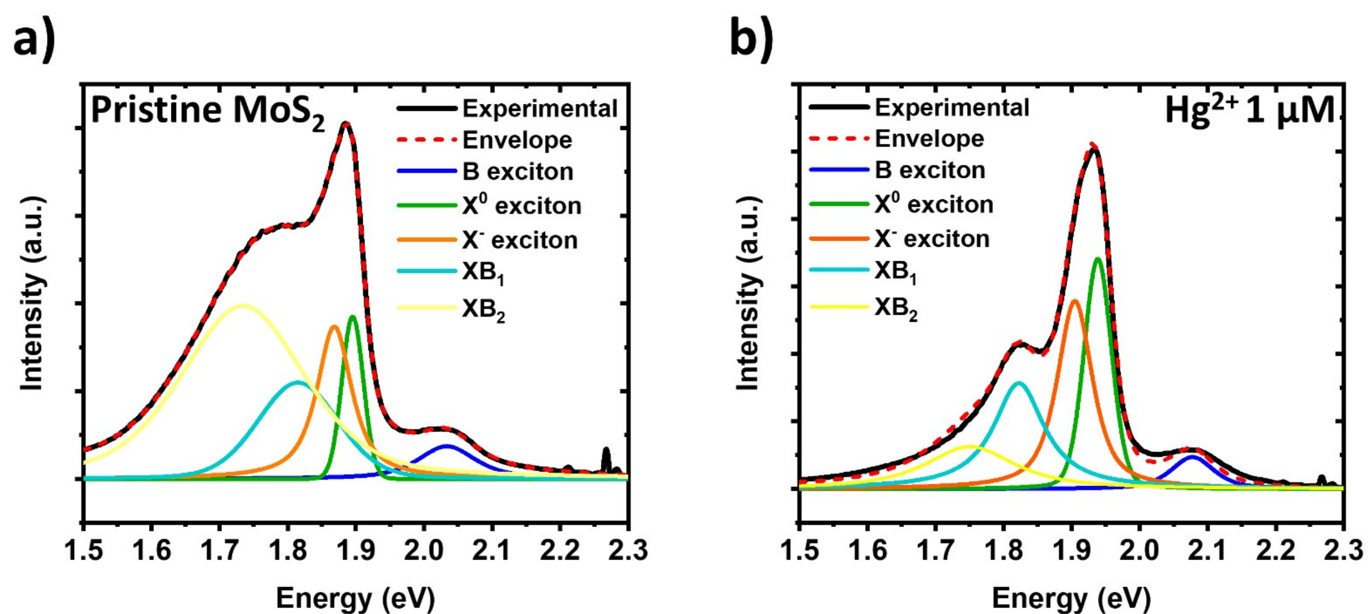

Fig S2. Low temperature PL characterization of CVD MoS_2 at different Hg^{2+} concentrations. **a)** Pristine CVD MoS_2. **b)** 1 µM exposed MoS_2. XB_1 and XB_2 bands' intensity, related to defects, strongly decreased after Hg^{2+} exposure, proving again defect healing. Neutral exciton band (X^0) increase after Hg^{2+} exposure. Both A and B exciton bands are blue-shifted. All these observations are in good accordance with the p-type doping observed in the electrical characterization.

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