Supporting information for

An Ultra-Sensitive and Recyclable FET-Type Toxic Gas Sensor

Based on WTe₂ Monolayer

Mi-Mi Dong^{1,2}, Hang He², Ming-Wen Zhao^{1*}, Chuan-Kui Wang^{2*}, Xiao-Xiao Fu^{2*}

¹ School of Physics, Shandong University, Jinan, 250100, China

² Shandong Key Laboratory of Medical Physics and Image Processing & Shandong

Provincial Engineering and Technical Center of Light Manipulations, School of Physics

and Electronics, Shandong Normal University, Jinan, 250358, China

*E-mail: zmw@sdu.edu.cn; ckwang@sdnu.edu.cn; fuxiaoxiao@sdnu.edu.cn



Fig. S1 Possible adsorption configurations and corresponding adsorption energies of the gas molecules adsorbed on the pure WTe₂ monolayer. The adsorption energy marked by blue color corresponds to the most stable adsorption configuration.



Fig. S2 Possible adsorption configurations and corresponding adsorption energies of the gas molecules adsorbed on the defectiveWTe₂ monolayer. The adsorption energy marked by blue color corresponds to the most stable adsorption configuration. The circles marked by black dashed lines mean the Te vacancies.



Fig. S3 (a) The phonon spectra of NO₂-defective WTe₂ adsorption system. (b) The phonon spectra of NO₂-defective WTe₂ adsorption system around the Fermi level.



Fig. S4 The Morse potential as function of the distance of the (a) pure WTe_2 and (b) defective WTe_2 adsorption systems.



Fig. S5 The spin-resolved current of the NO and NO₂ adsorbed pure WTe₂ FET-type gas sensors.