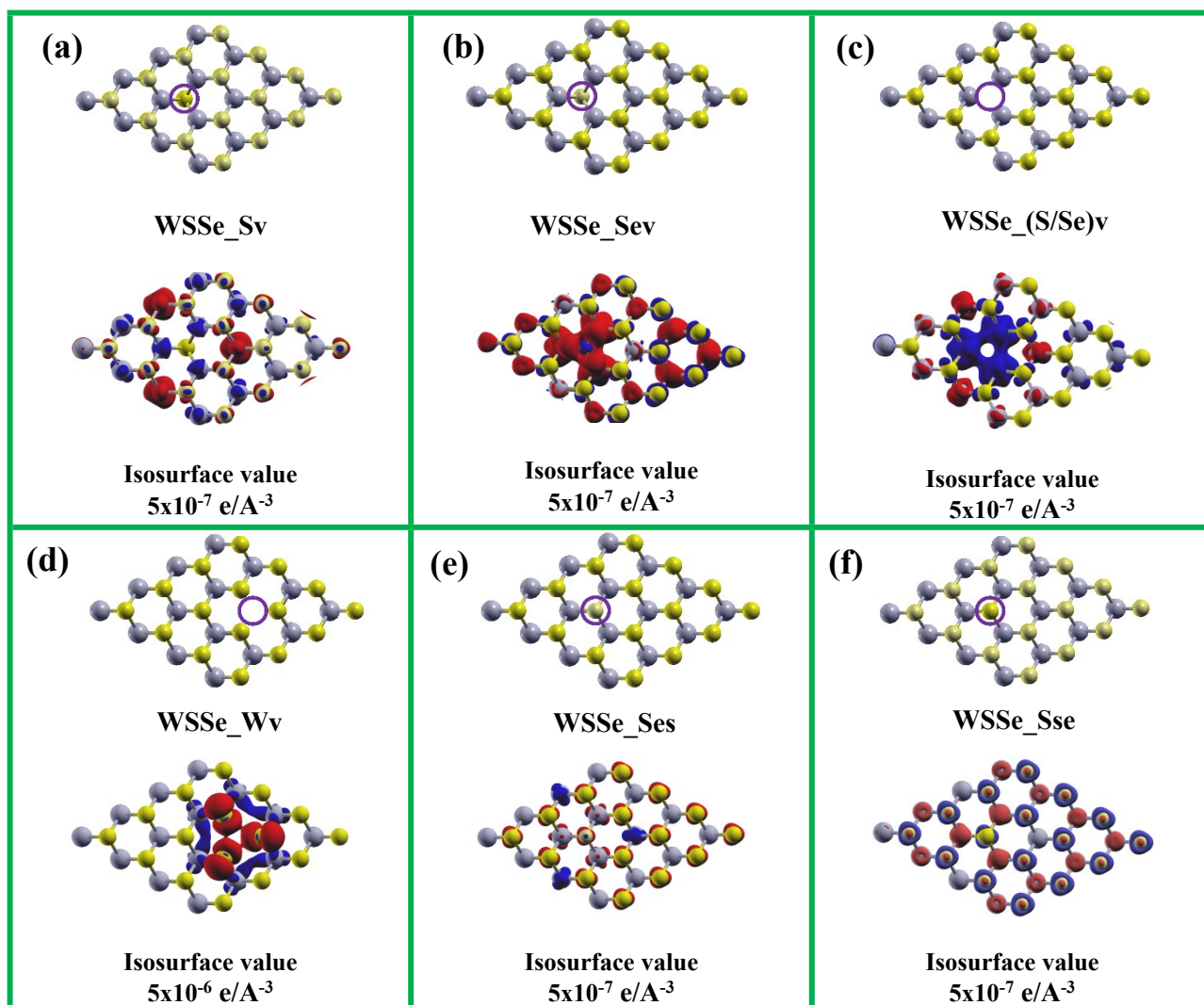


Supplementary Information:

Ultrahigh sensitivity with excellent recovery time for NH₃ and NO₂ in pristine and defect mediated Janus WSSe monolayer

Rajneesh Chaurasiya and Ambesh Dixit[#]

¹Department of Physics and Center for Solar Energy, Indian Institute of Technology Jodhpur, 342037, India
#ambesh@iitj.ac.in



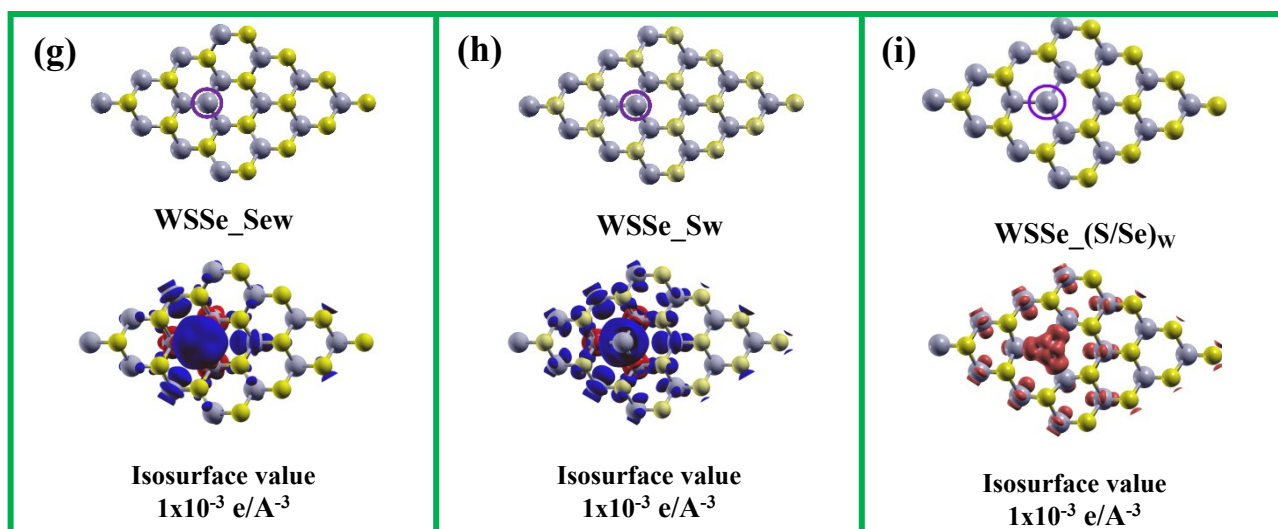


Figure S1: optimized structure and charge difference density of (a) sulfur vacancy (Sv), (b) selenium vacancy (Sev), (c) sulfur/selenium vacancy (S/Sev), (d) tungsten vacancy (Wv), (e) selenium replaced by sulfur atom (Ses), (f) sulfur replaced by selenium atom (Sse), (g) Selenium replaced by tungsten atom (Sew), (h) sulfur replaced by tungsten atom (Sw) and (i) sulfur/selenium replaced tungsten atom. Red color showing the negative charge while blue color showing the positive charge. (Purple color circle in the monolayer showing the position of defects)