Electronic Supplementary Material (ESI) for Materials Advances.

First principle study of WSe_2 and the effect of V doping on the optical and electronic properties

Eleonora Pavoni[a], Elaheh Mohebbi[a], Gian Marco Zampa[b], Pierluigi Stipa[a], Luca Pierantoni[b], Emiliano Laudadio[a]*, Davide Mencarelli[b]

Table S1. Bandgap energies calculated by using GGA-PBE and hybrid-HSE06.

Wse_2	**Bandgap obtained by GGA-PBE**	**Bandgap obtained by hybrid-HSE06**
Bulk undoped	0.94 eV (indirect), 1.58 eV (direct)	1.62 eV (indirect) 2.26 eV (direct)
1 ML undoped	1.68 eV (direct)	2.19 eV (direct)
1.4% of V doping	0.93 eV	
2.8% of V doping	0.91 eV	
5.6% of V doping	0.85 eV	
11.2% of V doping	0.80 eV	

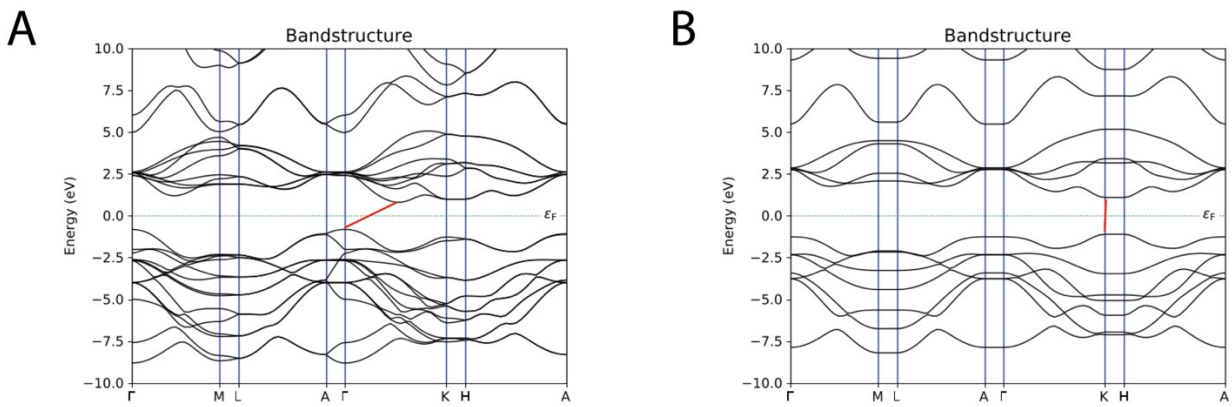

Fig. S1. Band structures of WSe_2 as (A) bulk material and as (B) a single layer calculated by using HybridGGA-HSE06 functional. The Fermi level is depicted as a dashed green line and the band gap as a red line.

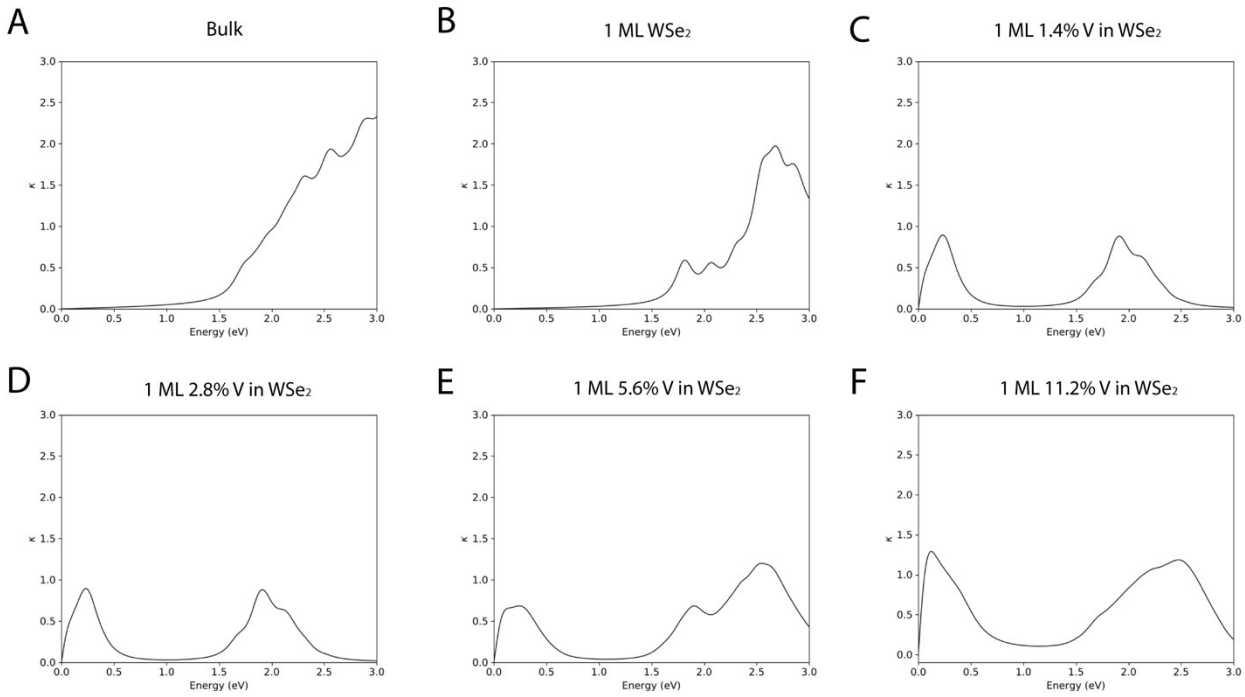

Fig. S2. Extinction coefficient spectra of WSe_2 as a bulk (A) and as 1ML (B). The extinction coefficient of WSe_2 doped with different percentages of V: WSe_2:V 1.4% (C), WSe_2:V 2.8% (D), WSe_2:V 5.6% (E), and WSe_2:V 11.2% (F). The spectra report the extinction coefficient (*k*) as a function of the energy, between 0 to 3 eV.

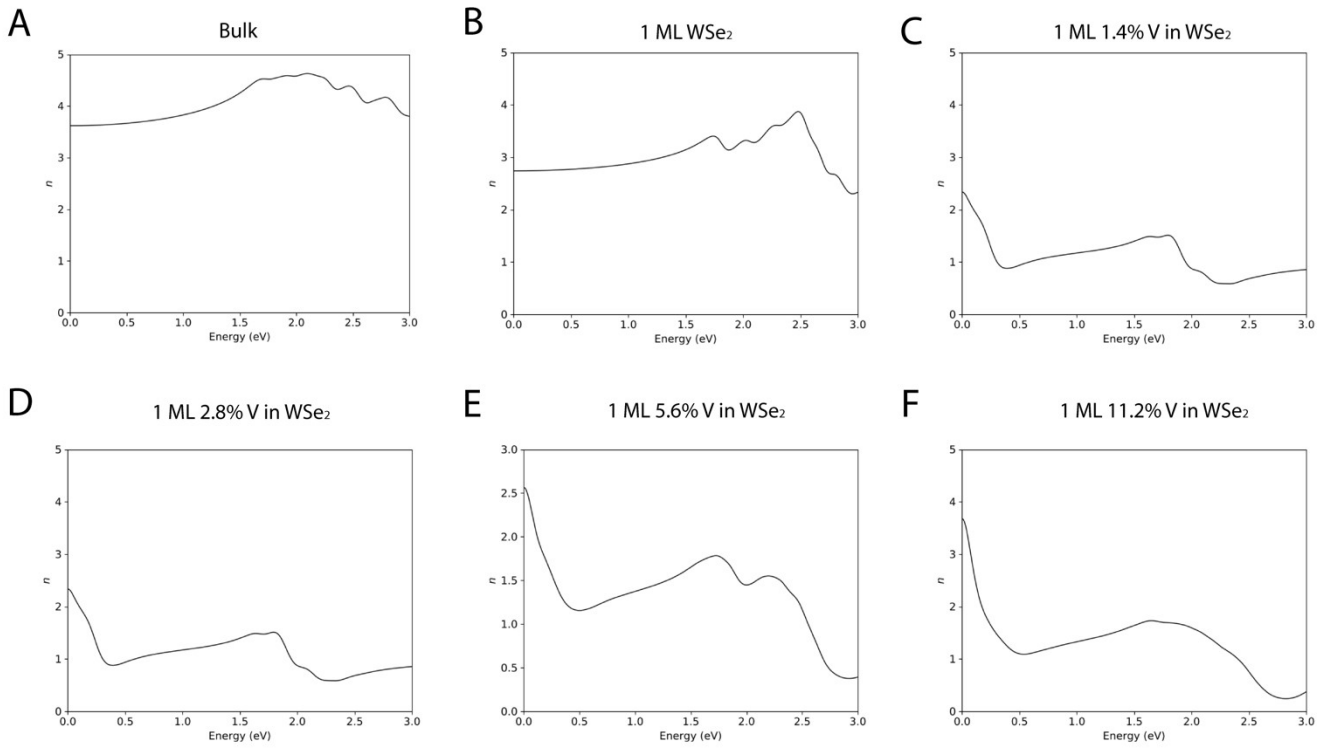

Fig. S3. Refractive index spectra of WSe_2 as a bulk (A) and as 1ML (B). Refractive index of WSe_2 doped with different percentages of V: WSe_2:V 1.4% (C), WSe_2:V 2.8% (D), WSe_2:V 5.6% (E), and WSe_2:V 11.2% (F). The spectra report the refractive index (*n*) as a function of the energy, between 0 to 3 eV.