Bound states induced by charged V dopants in monolayer WSe_2

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Besides exfolation of bulk van Waals crystals [1], substitutional doping of two-dimensional (2D) semiconductors of the family 1H-MX_2 (M=Mo or W, X=S or Se) by 3d metal atoms is an appealing approach to prepare 2D magnetic layers [2] at the wafer scale using thin films growth techniques. V is in principle a favourable case for doping owing to i) the prediction of a magnetic state [3] and ii) the demonstration of its incorporation at M sites [4]. We present here the analysis by STM/STS of the electronic structure of V doped WSe_2 samples grown by MBE on graphitized SiC surfaces. Individual V dopants show up as large circular structures with a strong electronic contrast (Fig. 1 a-b), which together with the observation of a local upwards band bending [5] demonstrates that the dopants are negatively charged. The associated electronic potential induces one bound state (in-gap sate) at the dopant site (Fig. 1 c). In line with this "electrostatic" picture, more strongly bound states appear for closely spaced V atoms. Charging is due to the band offset at the graphene/WSe_2 interface [6] and to the acceptor character of V atoms. Eventually, the excess charge would suppress the magnetic moment on the V atoms [4].

References

[1] C. Gong et al., Nature, 546 (2017) 265 ; B. Huang et al., Nature, 546 (2017) 270
[2] R. Mishra et al., Phys. Rev. B, 88 (2013) 144409
[3] N. Singh and U. Schwingenschlögl, Adv. Mater., 29 (2016) 1600970
[4] A. Robertson et al., ACS Nano, 10 (2016) 10227
[5] T. Le Quang et al., 2D Mater., 5 (2018) 035034
[6] T. Le Quang et al., 2D Mater., 4 (2017) 035019

Figures

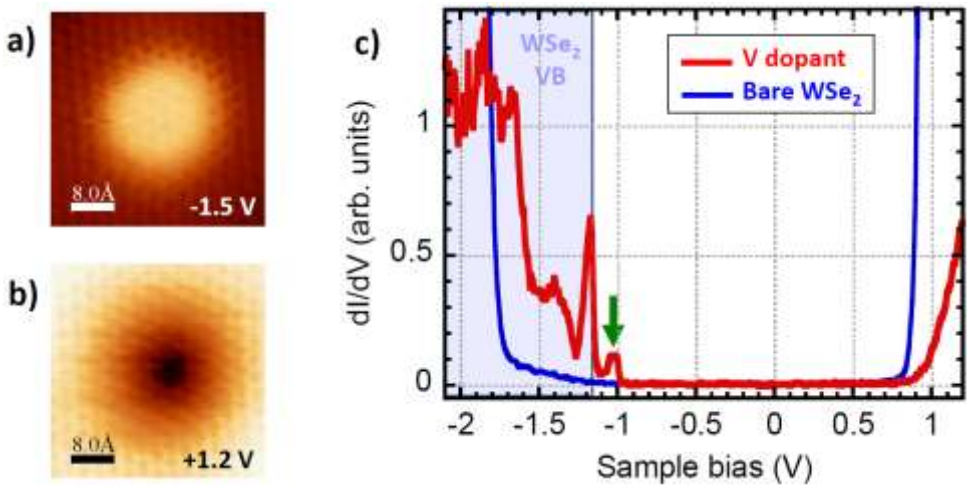

Figure 1: Electronic structure of isolated V dopants in monolayer WSe_2. a) and b) Constant current images of one dopant at negative (a) and positive (b) sample bias. c) Spectra taken at the site of a V dopant (red curve) and on a nearby bare WSe_2 spot (blue curve). The shaded area highlights the energy range of the valence band (VB) states of bare WSe_2. The green arrow points to the bound state systematically found at the V site, with 140 meV binding energy.