Detection of negative charge induced by single atom V dopants in 2D WSe_2 by 4D-STEM

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Structural anomalies in 2D materials have been known as the key to locally modify the electrical, optical and magnetic properties. In order to tailor the material properties and to explore their functionalities, the ability to survey the local electric properties together with their structural configuration at the atomic scale is essential. Recently, a new imaging technique called Center of Mass (CoM), sensitive to the local electrostatic field, has been demonstrated in a Scanning Transmission Electron Microscope (STEM) [1-2]. However, the lack of quantitative understanding and interpretation of CoM images is the main reason why this imaging mode is not yet routinely used for the study of 2D materials.

In this work, we explore the use of the CoM technique for atomic scale mapping of the local electrostatic field and potential around single atom V dopants in WSe_2/graphene heterostructure. The quantitative analysis is achieved by comparing the experimentally obtained E-field and potential maps to the Density Functional Theory based multislice STEM image simulations taking into account the influence of important microscope parameters such as: convergence angle, defocus and lens aberrations. A negative charge around V dopants is detected as a drop in the electrostatic potential maps (Fig. 1A).

Finally, the technique was used for imaging the electrostatic potential landscape in complex structural configurations in the presence of growth related defects such as Se vacancies, inversion domain boundaries (Fig. 1B), opening the perspective for atomic scale analysis of charge effects and interactions between charged defects in synthesized 2D materials [3].

References

[1] N. Shibata et al., Nature Physics, 8 (2012) 611
[2] K. Müller et al., Nature Communications, 5 (2014) 5653
[3] D. Dosenovic et al, ACS Nano (under review)

Figures

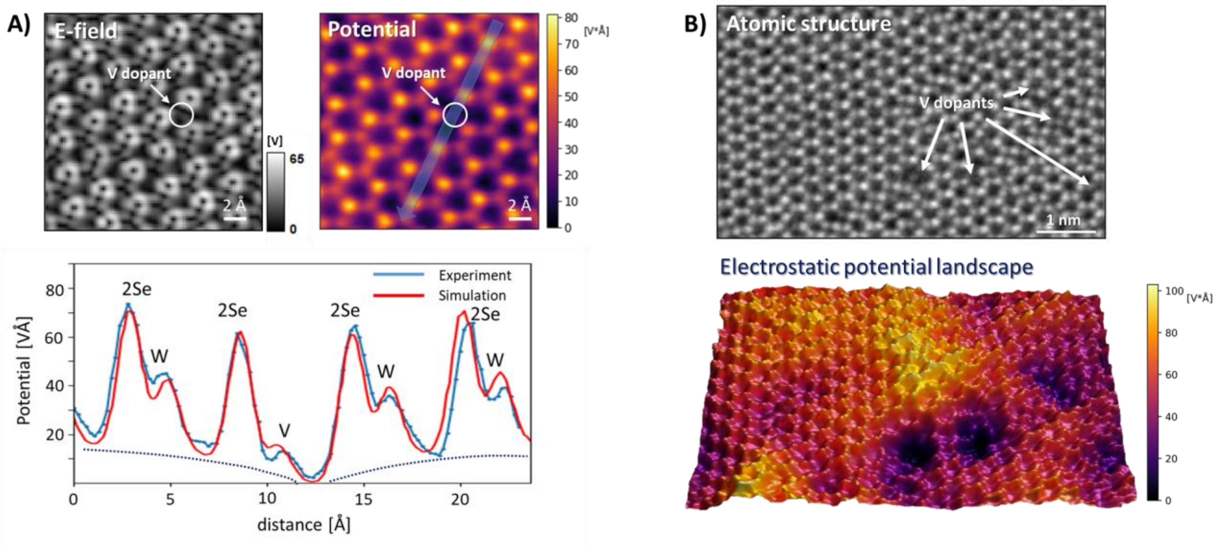

Figure 1: A) Experimental projected E- field and potential around single V dopant atom compared with DFT-based simulations on a negatively charged V dopant. B) Electrostatic potential landscape around complex defect configurations.