Real space Kubo-Greenwood simulations for charge transport in MoS_2: Impact of sulphur vacancies.

Sai Manoj Gali[1], Anton Pershin[1], Aurélien Lherbier[2], Jean-Christophe Charlier[2] and David Beljonne[1].

[1]*Laboratory for Chemistry of Novel Materials, University of Mons, Mons, Belgium*
[2]*Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve, Belgium.*

Contact@E-mail saimanoj.gali@umons.ac.be

Imperfections, such as point defects, in two dimensional (2D) materials can modulate their charge transport characteristics [1-2]. The impact of point defects of the form of 'sulfur' vacancies in single layers of MoS_2, a semiconducting transition metal dichalcogenide (TMDC) material, are investigated theoretically. The real space order-N Kubo-Greenwood (KG) transport mechanism [1-2] is employed with the sp^3d^5 orthogonal tight binding (oTB) parameters derived for MoS_2 monolayer in its pristine form and with sulfur vacancies of upto 3 % vacancy concentration by considering the electronic structure with in six bands. The sulfur vacancies are placed either on one side or two sides of the monolaye, randomly arranged and with a user-defined spatial correlation (see Fig: 1). The band mobilities of MoS_2 as a function of sulfur vacancies were computed. The band mobilities obtained from the KG simulations (see Fig: 2) are in good agreement when compared with the experimental and also with the band and field effect mobilities from the previous studies [3].

References

[1] A. Lherbier et al, Phys. Rev. B., 87 (2013), 195448.
[2] Gargiulo et al, Phys. Rev. Lett., 113 (2014), 246601.
[3] Bertolazzi et al, Adv. Mat., 29 (2017), 1606760.

Figures

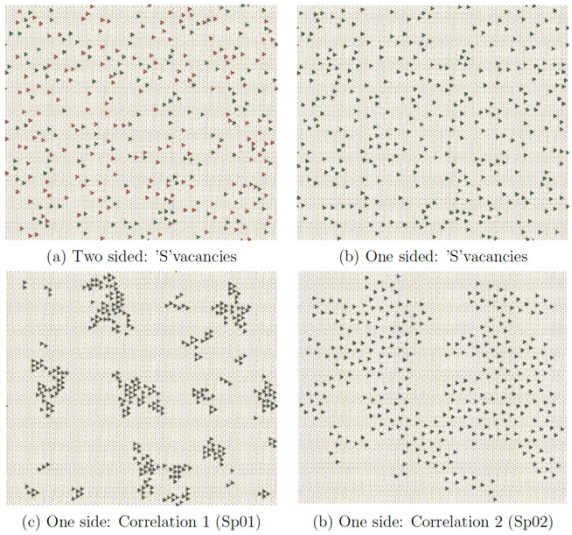

Figure 1: Atomic positions of MoS_2 monolayer with 1.5 % 'S' vacancies. Sulfur vacancies on one side of the monolayer are represented by green and those on the other side by red. Top: random vacancies and bottom: sulfur vacancies with correlation.

Figure 2: Comparison to experimental mobilities (Exp). Calculated band and field effect mobilities are represented by 'B' and 'F', while 'BT' and 'KG' stand for semi-classical Boltzmann transport and KG simulation schemes, respectively.