The mystery of semiconductor to metal phase transition in MoS_2 under electron beam

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Recently a phase transition from the hexagonal 1H to trigonal distorted 1T'-phase in two-dimensional (2D) MoS_2 has been induced by electron irradiation [1]. Using density functional theory calculations, we study the energetics of these stable and metastable phases when electric charge, mechanical strain and vacancies are present. Based on the results of our calculations, we propose an explanation for this phenomenon which is likely promoted by charge redistribution in the monolayer combined with vacancy formation due to electron beam and associated mechanical strain in the sample.

References

[1] Y.-C. Lin, D. O. Dumcenco, Y.-S. Huang, and K. Suenaga, Nature Nanotechnology 9 (2014) 391

Figures

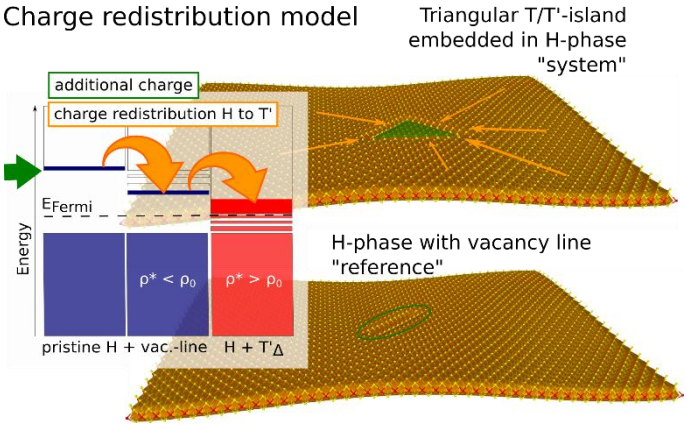

Figure 1. Additional charge initially located in the conduction band minimum is redistributed to the triangular metallic region. This causes the configuration with the metallic region to become energetically favorable over the semiconducting reference configuration with vacancy line.