Phase Transitions in Two-Dimensional Transition Metal Dichalcogenides 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. We further show that this mechanism can be extended to other 2D transition metal dichalcogenides.

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