

# **First Principle Studies of Point Charge Defect in Two Dimensional Materials**

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Vacancies, adatoms, dopants, and interstitials change the electronic and optical properties of materials. These defects can be charge neutral; however, some defects can have a net charge. The computational modeling of formation, movement, and combination of charged defects will allow us to study doping of materials in the newly discovered family of two-dimensional materials for use in devices such as solar cells, light-emitting diodes, or transistors. However, theoretical study of charged defects presents challenges and introduces electrostatics artifacts. In this study, we calculate formation energies of charged defects in two-dimensional materials using correction method that is based on a surrogate model for the electrostatics.