Simulated doping: from space charge regions to 2d materials

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Abstract

Doping is an essential and indispensable part of semiconductor technology. However, the inclusion of the global effects of semiconductor doping poses a unique challenge for first-principles simulations, because the typically low concentration of dopants renders an explicit treatment intractable. Here, I will present a simple yet effective approach based on "pseudoatoms", possessing a fractional nuclear charge matching the bulk doping concentration. For simulating space charge regions, the approach is augmented by a multiscale technique that is based on the introduction of a charged sheet, mimicking the SCR-related field, along with free charge which mimics the bulk charge reservoir, such that the system is neutral overall. I will show a wide range of scenarios where this approach is useful, including recent applications to novel polarization phenomena in 2d materials.