

Abstract Submitted
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Dopant Induced Stress and Strain Enhanced Doping¹ JUNYI ZHU, SUHUI WEI, National Renewable Energy Laboratory, GERALD STRINGFELLOW, FENG LIU, University of Utah — We report an intriguing dopant induced electronic stress effect. A foreign dopant atom induces a lattice stress. Conventional dopant induced stress is due to the different atomic sizes between the dopant and host element. Here, we discovered an intriguing dopant induced electronic stress effect. First principles calculation reveals that even a dopant with the same atomic size as the host atom induces a lattice stress of electronic origin, because it has either one more or one less electron than the host. We also found that the electronic stress exhibits a nonlinear dependence on strain, different from the conventional atomic stress effect. In general, the competition between the atomic stress and electronic stress determines the overall stress induced by a dopant, which in turn determines how external strain will change the doping energy.

¹We thank Zheng Liu for his useful discussions. The calculations were performed on AMD Opteron cluster at the CHPC, University of Utah and on the Franklin cluster at National Energy Research Scientific Computing Center.

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