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Electronic structures and work functions of InN(0001) films[1]
JUNG-HWAN SONG, ARTHUR J. FREEMAN, Northwestern U. — InN films have attracted great attention with its recently discovered band gap, 0.7eV, and evidence for p-type doping[2]. We have studied theoretically the electronic structures, surfaces, and work functions of InN films using the highly precise FLAPW method[3]. The passivation with pseudo-hydrogens[4] has also been applied to the surfaces of InN(0001) films for comparison with the electronic structure of the ideal InN(0001) films. We compare the work functions of InN films with other wurtzite materials such as ZnO, GaN, and AlN, which we have also calculated. We discuss the mechanism of the structural transition[5] with layer thickness for the very thin InN(0001) films, for which we have found that the ideal InN(0001) films of the wurtzite structure, up to 4 bilayers, optimize to the graphitic- like structure. We then discuss the relationship between the dipoles and the surfaces (work functions) of the InN(0001) films, and the possibilities of their p-type doping.

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Jung-Hwan Song
Northwestern University

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