First-principles model of absolute band shifts induced by (001) biaxial strain in group IIIA-VA semiconductors EUGENE KADANTSEV, PAWEL HAWRYLAK, IMS NRC — A new model for the evolution of conduction and valence bands of IIIA-VA (InAs, GaAs, InP) semiconductors under (001) biaxial strain is developed. The model is based on ab initio calculations which take into account finite strain dependent relaxation of the reference levels. It is shown that in type I heterostructures subjected to (001) compressive biaxial strain, the confinement of holes can be reduced as compared to some existing models of biaxial strain.

Pawel Hawrylak
IMS NRC

Date submitted: 15 Nov 2010  
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