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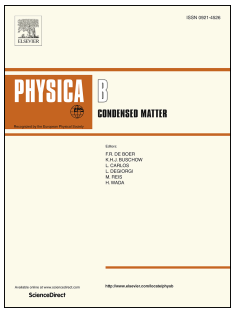

Conduction-and valence band offsets of $Zn_{1-x}Mg_xSe/Zn_{1-y}Mg_ySe$ heterointerfaces

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Conduction-and valence band offsets of $Zn_{1-x}Mg_xSe/Zn_{1-y}Mg_ySe$ heterointerfaces

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Abstract

Based on the model-solid theory coupled with a pseudopotential approach within the virtual crystal approximation, the conduction and valence band offsets (CBO) and (VBO) of the unstrained and strained $Zn_{1-x}Mg_xSe/Zn_{1-y}Mg_ySe$ heterointerfaces have been investigated. The calculated elastic constants C_{11} and C_{12} for ZnSe and MgSe are found to agree to within 7% with experiment. Our findings showed that for electrons the CBO is negative whereas the Mg content of the overlayer (x) is lower than the Mg content of the substrate (y). Nevertheless, the reverse can be seen when x > y. As regards the light-and heavy holes the VBOs remain negative as far as the Mg concentration of the overlayer is lower than that of substrate layers and become positive in the opposite case. The alignment of the bands is found to be of type II (staggered) whatever is the Mg compositions of both the overlayer and the substrate layer. The relaxed and strained band-gap energies versus the composition y have been computed and the results are examined and discussed.