











FIG. 3. Energy band structure of ZB (solid line) and rhombohedral (RH) SiGe (dashed line) as functions of the lattice constant  $a$  for  $a_{\text{Si}} = 0.357 \text{ nm}$  and  $a_{\text{Ge}} = 0.357 \text{ nm}$ . For rhombohedral SiGe, the energy scale was adjusted such that the minimum of the curve gives the enthalpy of formation.  $\Delta E_{\text{ss}}$  denotes the substrate strain. The shaded area denotes the negative enthalpy of formation. Energy value of 0 eV was used.