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New optical transitions in strained Si-Ge superlattices

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First-principles total-energy and electronic-structure calculations for Si„Ge„superlattices grown

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(e) (d) (c) (1) {a)
Si SIo.s Qeo.s
asl
c/a = 1

', (c/a)eq
2.0— 'I
rc

Qe Ge Qe
asi asi aGe

(c/a)eq c/a = 1 c/a = 1

1.5—Lc

4P

1.0—

O
C
UJ

05—

Lc
xc

&c

r.(
n

xc
Lc

xc

xc

Lc

O ~ Il r„~" r„

FIG. 1. (a) Energy levels (in eV, relative to the average of the strain-split valence-band maximum states) at I, X, and L of (a) bulk Ge (ao, 5.61 A) and (e) Si (as;=5.41 A), as well as (d)
distorted Ge [(b) and (c)] and a Si05Geo q alloy (aa~,„=5.51 A).

and [010] directions) splits the six A; conduction-band valleys of Ge into two, degenerate longitudinal states A; and four, degenerate transverse states A; [Fig. 1(c)l. For (c/a) & 1 (appropriate here) the A; states shift to higher
energy relative to A (a splitting of 0.5 eV for Ge). In
contrast, since the Ge conduction-band valleys at I, are
oriented along the

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