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Comment on "Electronic Structure and Optical
Properties of Si-Ge Superlattices" Ge
~SI

Si
~SI

Si4 Ge4
Sl

Si4 Ge4
~Ge

Si
~Ge

Ge
~Ge

(e) (I)

We have self-consistently calculated' the electronic
structure of the strained Si4Ge4/Si(001) superlattice, in-
terpreting the electrorellectance transitions A (observed
1.24 eV, calculated 1.26 eV) and B (observed 1.8 eV,
calculated 1.74 eV) as folded-in (pseudo) direct excita-
tions [Figs. 1(a)-1(c)], in accord with Ref. 2. In con-
trast, transition I, observed at 0.8 eV and interpreted pre-
viously as the direct band gap, was shown to be an in-
direct I,, h,, excitation either to the superlattice 6,,
state (calculated' at 0.92 eV) or to the substrate d„state (calculated at 0.80 eV). Other calculations and experi-ments support this assignment. More recently, Wong et
al. carried out non-self-consistent calculations within
the empirical pseudopotential method. The central point
of their Letter was to note that if larger Ge-Ge interpla-
nar spacings were postulated (making the Ge —Ge bond
lengths longer and more bulklike), the direct superlattice band gap (transition A) was reduced from 1.2 to 0.9 eV, close to the value where transition I was seen. On the
basis of this empirical adjustment, they proposed that

the observed transition I is in fact the direct band gap
(A), in conllict with more recent experiments. " This pa-
rameter adjustment was not constrained by any (varia-
tional or microscopic) principle; the only motivation was that it might mimic eA'ects of defects at Si/Ge interfaces. However, such interfacial defects are more likely to des-troy coherence with the substrate, removing the biaxial
epitaxial constraint (a~~ =as;), than to permit uniaxial
relaxation of Ge—Ge bonds. In both cases Ge—Ge bonds relax, but in the former the Ge-Ge interplanar dis-
tance naturally becomes smaller. We show below that
(i) even if the assumed increase in Ge-Ge interplanar