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Absolute deformation potentials of Al, Si, and NaC1 Alberto Franceschetti, Su-Huai Wei, and Alex

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tial by singling out the effect of atomic size differences,
these authors obtain the deformation potential of the
CBM of Si for (001)strain.
A number of theoretical approaches have been applied
to the deformation potential problem. The simple tight-
binding model of Harrison,

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assuming arbitrarily that
the diagonal matrix elements of the Hamiltonian (atomic-orbital energies) are volume

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used the value /=0. 53 obtained by Nielsen and Martin. ' The crystal-field averaged ADP of the valence-band max-

imum (sometimes denoted by a„)is compared in Table I
with the previous ab initio calculations of Van de %alle and Martin and of Resta, Colornbo and Baroni, and with the experimental results of Cargill, Angilello, and Kavanagh. As we can see, the agreement is quite good for the (001) and (111)directions. In the case of the (110) direction, our result is probably affected by the slow con-vergence of the ADP with respect to the dimension of the
supercell. '
The ADP's of a simple metal (Al), a semiconductor (Si), and an insulator (NaC1) are shown in Fig. 2 for (001) uniaxial strain. Note that the (001} interface of the compressed-expanded homojunction of NaCl is nonpolar;
therefore, the displacement of the interfacial atomic
planes in the direction of the strain does not change the ADP A.lthough the energy gaps shown in Fig 2a.re not to scale, the slopes of the lines (absolute deformation po-tentials) are plotted to scale, so that the ADP's of different states and different materials can be directly compared. The following