VOLUME 70, NUMBER 11 PH YSICAL REVI EW LETTERS 15 MARCH 1993 OH'-Center Atomic Displacements in Zinc-Blende Semiconductoic

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Q=0.OO Q=0.16

a, (X,,)

a|(I'1,

'I 5d

~+~)
FIG. 3. Charge density contour p1ots for the CuC1 states of

Fig. 2(a) at Q =0 and 0.16.

ed CuC1 the VB maximum is the threefold degenerate t2d(I lsd) state; the empty CB minimum is a al(I l,) s-like state. As the Cu atom is displaced towards the trigo-nal face, the al

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CL) 5.2
LLJ

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