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E , L , G , , C 80401, A
(g2/F51Tf16.34070TD(B)Tj/F41Tf0.65890TD(2)Tj/F21Tf0.49720TD[()-385.8(has)-387.1(its)]TJ/F41Tf3

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Li, the $hR1$ structure transforms to the $cI16$ structure at about 35 GPa, then at about 75 GPa it transforms to the $C2$ structure, and then at about 98 GPa it transforms to the $Aba2$ structure, which persists up to at least 160 GPa; for Cs, the $Cmca$ structure transforms to the $dhcp$ structure at about 60 GPa, which persists up to at least 200 GPa. The transition pressures are in agreement with the experimental results [3 5]. Random search techniques [24] and the evolutionary algorithm method [25,26] were previously applied to search the ground states of elemental lithium

$$\Delta H_{VD} = [H(Li, V_m) - H(Li, V_1)] + [H(Cs, V_m) - H(Cs, V_2)]. \tag{1}$$

The charge-transfer energy ΔH_{CT} is the enthalpy change when combining bcc Cs and bcc Li at the constant-volume V_m to form LiCs ($B2$),

$$\Delta H_{CT} = H(LiCs, V_m) - H(Li, V_m) - H(Cs, V_m). \tag{2}$$

ΔH_{VD} and ΔH_{CT} are shown as the red line and the green line in Fig. 4(a), respectively. We see that ΔH_{VD} is positive and increases rapidly as pressure increases, the main effect coming from the $P(V_2 - V_1)/2$ term (dashed line). At zero pressure, ΔH_{VD} ($\simeq 520$ meV/atom) is large enough to make the Li-Cs system phase separating. In contrast, ΔH_{CT} is negative and decreases rapidly as pressure increases. At 160 GPa, $\Delta H = -238$ meV/atom and ΔH_{CT} is large enough to induce ordering in Li-Cs.

The electronic structures of LiCs ($B2$) are shown in Figs. 4(b) and 4(c). At zero pressure the dispersions of the Li(1s), Cs(5s), and Cs(5p) bands are all small. At 160 GPa, the Li(1s) band still has negligible dispersion, while the dispersion of the Cs(5s)

high-pressure compounds bet een t o elements in the same column of the periodic table (Li-Cs) is perhaps reminiscent of compound formation and charge transfer bet een Ag-K [27] or Li-Be [17], although the latter t o cases are perhaps less surprising than Li-Cs as the repre- sent a far larger chemical disparit (hence, reactivit) bet een the constituent elements that belong to different columns in the periodic table.

Li$_7$Cs (*Cmmm*) ^{x} , , 1D- , , , . The electronic structure of Li$_7$Cs (*Cmmm*) at 80 GPa e hibits interesting features of 1D-like bands. Its densit of states at the Csð5sÞ and Csð5pÞ bands [see Fig. 6(a)] displa s a remarkable feature of t pical 1D electronic structure, the emergence of hich in a three-dimensional environment is rather une - pected. Figure 6(b) sho s the band structure of Li$_7$Cs (*Cmmm*) at 80 GPa. The Csð5sÞ and Csð5pÞ bands displa strong dispersion onl along the Γ-X_3 direction, but are nearl dispersionless along other directions. The 1D band structure is caused b the unique cr stal structure of Li$_7$Cs (*Cmmm*) [see the inset of Fig. 3(a)]. The Cs chains are embedded in the three-dimensional Li net orks and are separated from each other. Along the chain direction, the Cs atoms are close to each other and their cores overlap.