in this series is displayed in Figure 3, which used a lattice parameter reduced 3% from the value used for Figure 2. Now the band gap for Figure 2 was adjusted to obtain a value of 0.63 eV by variation of the exchange multiplier $\alpha$; however, without any further variation of $\alpha$, the band gap of Figure 3 has been reduced to 0.10 eV. Thus, it is seen that lattice parameter reduction decreases the calculated band gap for SmTe. The calculated band gap for SmTe as a function of lattice parameter is given by Figure 4. From this figure it is seen that the calculations indicate, as discussed earlier, that the application of pressure causes SmTe's band structure to continuously undergo a transition from the type illustrated by Figure 1(b) to the type illustrated by Figure 1(c). Also, the data of Figure 4 indicate the calculated semiconductor-to-metal transition occurs when the lattice parameter has been reduced by about 3.5%. Without the availability of detailed compressibility data for SmTe, it is not possible to express what pressure the calculations predict for the transition. However, Rooymans[15] has reported SmTe lattice constants of 12.3 a.u. at 30 kbar and 11.7 a.u. at 60 kbar. So the calculated transition pressure falls approximately halfway between 30 and 60 kbar, which, when considering the approximations used in the calculations, gives very reasonable agreement with the experimental[10] transition pressure of about 50 kbar.

We have also performed calculations pertaining to SmS using similar procedures as those used for SmTe. First, using the normal pressure lattice parameter (cube edge = 11.28 a.u.), the value of the exchange multiplier $\alpha$ was varied until the calculated gap between occupied states and the conduction band agreed with the experimental absorption edge of about 0.2 eV. For SmS, as is seen from Figure 5, in order to obtain agreement the calculational process led to the presence of the f-states between the valence and conduction bands. To further illustrate this point, for $\alpha = 1.00$ the gap between the valence and conduction bands was 2.9 eV with the f-states considerably below the valence band, for $\alpha = 0.90$ the valence-conduction gap was 2.3 eV and the f-states were still below but closer to the valence band, and for $\alpha = 0.80$ the valence-conduction gap was also 2.3 eV but the f-states had moved between the valence and conduction bands. Final adjustment gave $\alpha = 0.781$ and the band structure of Figure 5, which has a valence-conduction gap of 1.9 eV but an f-state to conduction band gap of 0.22 eV. Thus, our calculations indicate that indeed SmS has a band structure of the type illustrated by Figure 1(a), as had been postulated by Jayaraman et al.[10]

To further test the validity of the calculational procedures, we performed a series of calculations for SmS with $\alpha$ fixed at the above final value of 0.781 but varied the lattice parameter. Part of the resulting band structure for a 2% reduction in lattice parameter is shown in Figure 6. It is seen for this compression, which is equivalent to a pressure of 6 kbar,[10] that the tail of the $\Delta_2'$ band has merged with the f-states, and providing 4f delocalization then occurs the system will be metallic. Since the observed transition pressure for SmS is 6.5 kbar, the agreement between our



calculations and experiment is quite reasonable.

In summary, our calculations strongly indicate that the mechanism for the pressure-induced semiconductor-to-metal transition in SmS is 4f electron delocalization, but the mechanism for SmTe (as for SmSe) is one involving simple closing of the valence to conduction band gap with pressure. If indeed such is the actual case, the experimental fact that the transition appears discontinuous for SmS and continuous for SmTe is not so mysterious.

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