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R. Sinclair

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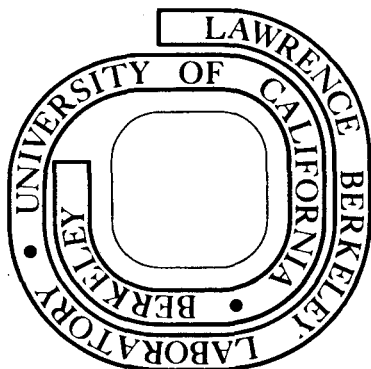
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EMPIRICAL RELATION BETWEEN ENERGY GAP AND LATTICE CONSTANT
IN CUBIC SEMICONDUCTORS

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ABSTRACT

The empirical relation $E_0 \propto (1/a_0^2)$ between the energy gap E_0 and lattice constant a_0 has been found to hold for a wide range of semiconductors with the cubic NaCl crystal structure.

In a previous letter¹, an empirical relation between the energy gap E_0 and lattice constant a_0 of cubic (NaCl structure) semiconductors was applied to PbS, PbSe, PbTe, and PbPo. This relation, which states that E_0 is directly proportional to $(1/a_0^2)$ for a series of related semiconductors, was known² to hold reasonably well for the group IV elemental semiconductors. The purpose of this addendum is to show that this empirical relation holds for a large number of semiconductors with the NaCl f.c.c. crystal structure.

Values³ of energy gap E_0 were plotted as a function of $(1/a_0^2)$ for the following sequences of related semiconductors: (1) BaS, BaSe, BaTe; (2) CaS, CaSe, CaTe; (3) SrS, SrSe, SrTe; (4) solid solutions of SnTe in PbTe; (5) solid solutions of SnSe in PbSe. The results for sequences (1) - (4) are shown in Figures 1 and 2 below; the result for sequence (5) is shown in the letter¹ mentioned above.

For all five sequences of semiconductors with the NaCl structure, the empirical relation $E_0 \propto (1/a_0^2)$ is well satisfied. It is of particular interest that the data for solid solutions of SnSe in PbSe cover both positive and negative values of $E_0 \equiv E(L_6^-) - E(L_6^+)$. For this reason, it is also of interest to note that this empirical relation holds also for CdTe⁴, for HgTe⁵, and for solid solutions⁶⁻⁹ $\text{Hg}_{(1-x)}\text{Cd}_x\text{Te}$ ($0.86 \geq x \geq 0.63$, zinc blende structure) with both positive and negative values of the energy gap $E_G \equiv E(\Gamma_6) - E(\Gamma_8)$. This result is shown in Figure 3.

In summary, this empirical relation $E_0 \propto (1/a_0^2)$ has been found to hold for a wide range of semiconductors with the NaCl structure with both positive and negative energy gaps. This result has been used, in results published elsewhere^{1,10}, to investigate the PbS group of semiconductors, including lead polonide (PbPo).

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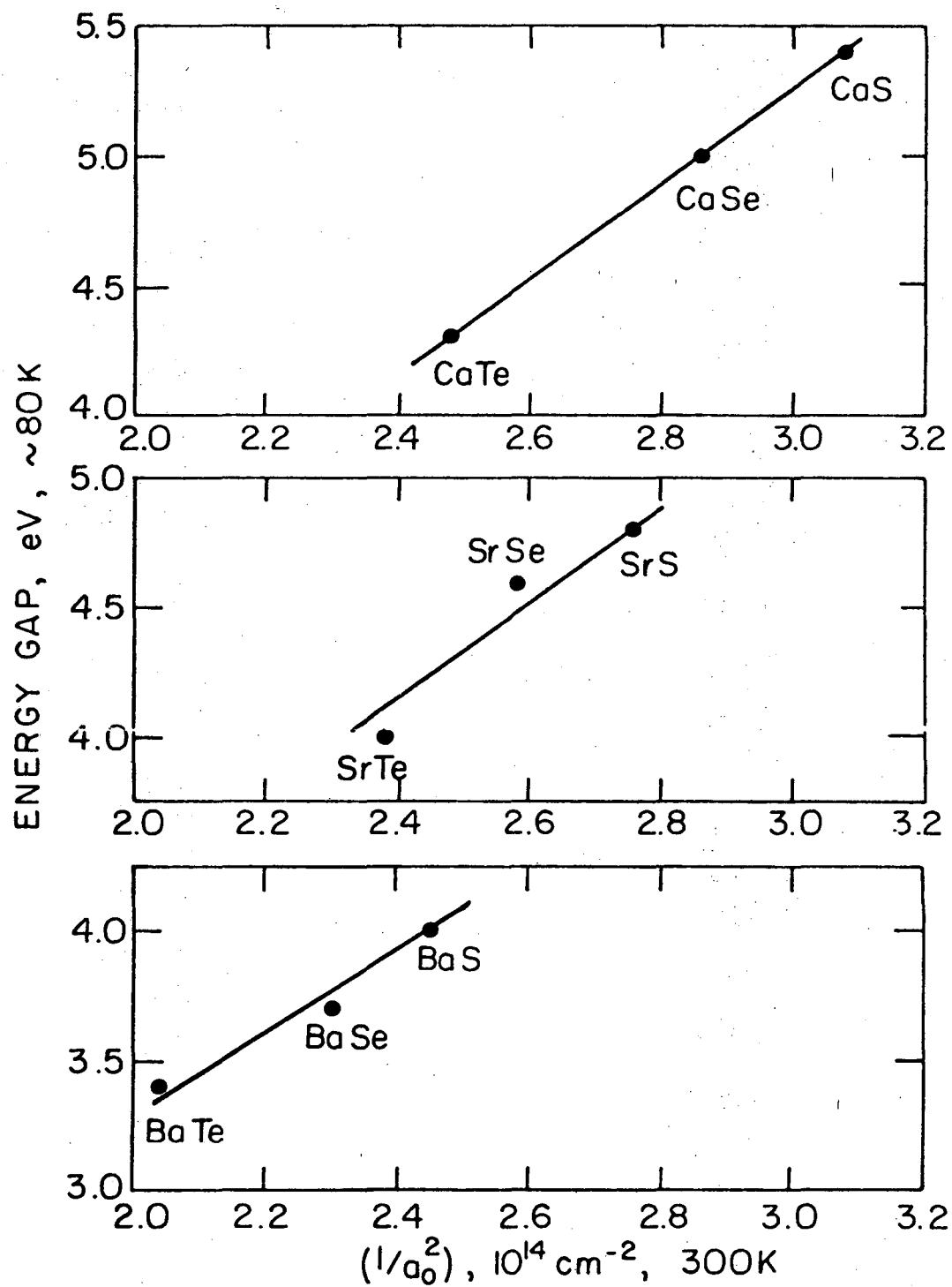
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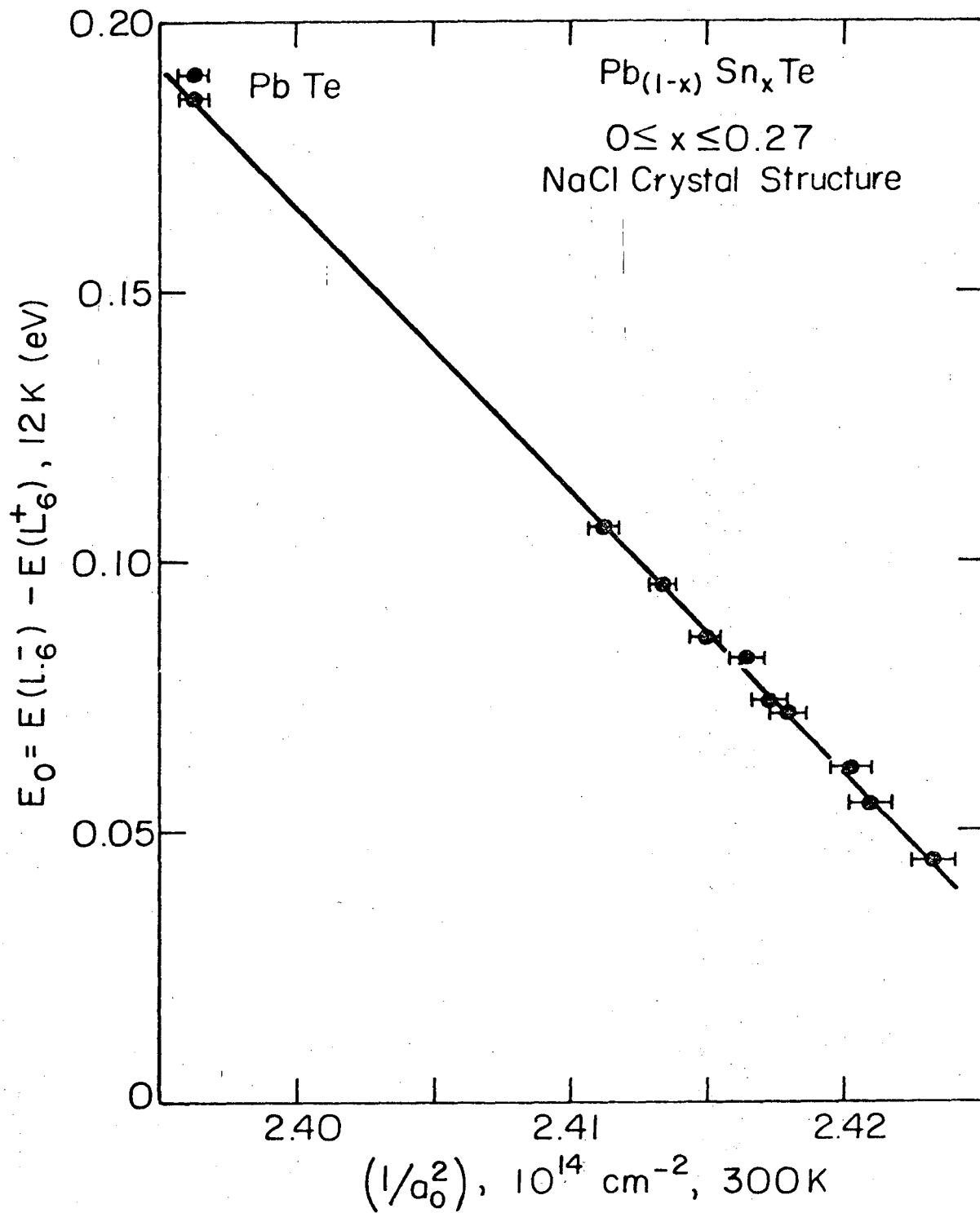
FIGURE CAPTIONS

- Figure 1. Energy gap plotted as a function of $(1/a_o^2)$ for CaS, CaSe, CaTe; SrS, SrSe, SrTe; BaS, BaSe, BaTe.
- Figure 2. Energy gap E_o plotted as a function of $(1/a_o^2)$ for solid solutions of SnTe in PbTe.
- Figure 3. Energy gap $E_G \equiv E(\Gamma_6) - E(\Gamma_8)$ plotted as a function of $(1/a_o^2)$ for solid solutions of HgTe in CdTe.



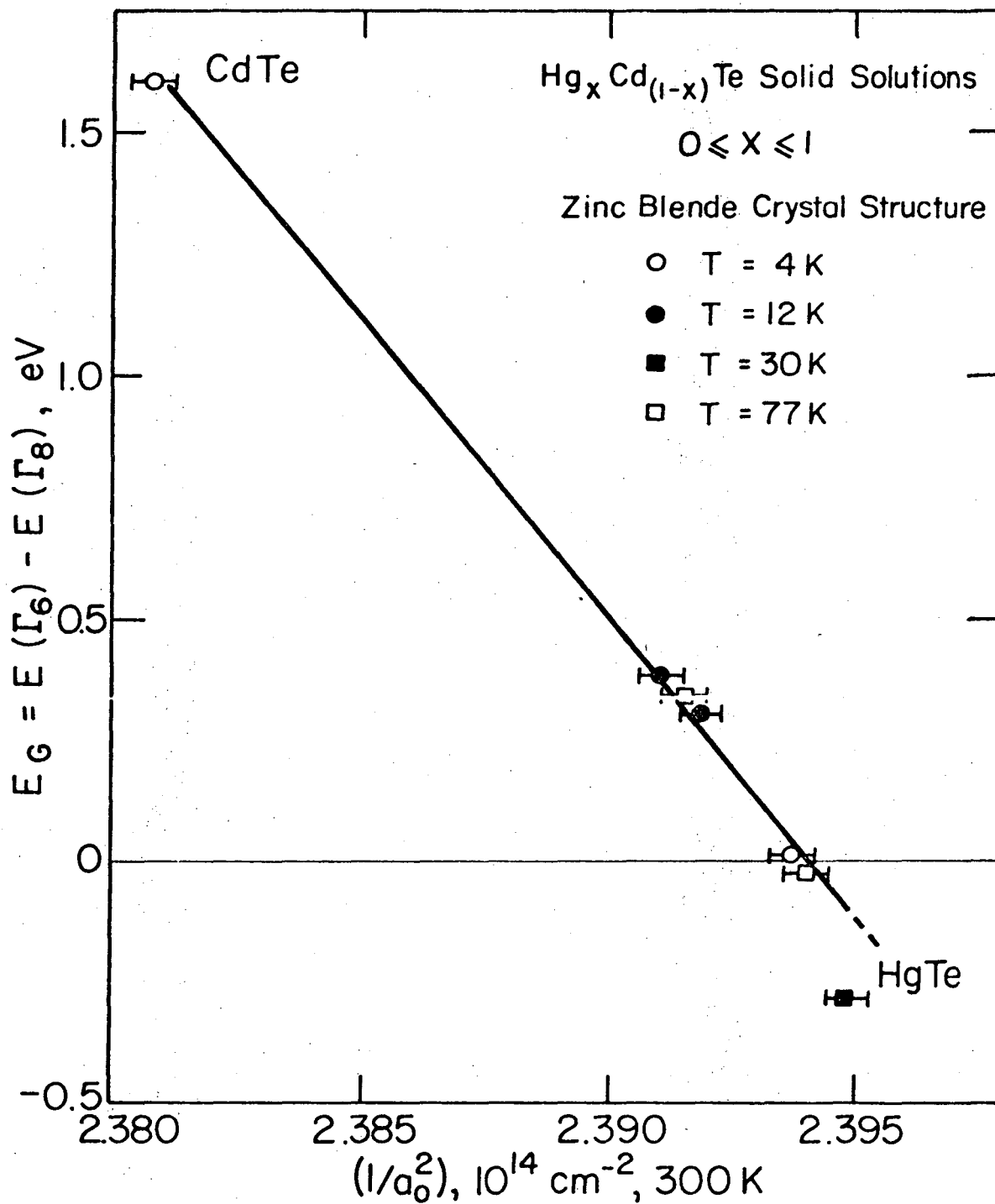
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Fig. 1



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Fig. 2



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Fig. 3

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