

Origins of Nonstoichiometry and Vacancy Ordering in $\text{Sc}_{1-x}\square_x\text{S}$

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... D ... (: , ...),
 ... B ...
 ... (111) ... (112)
 ... E ...
 ... $\sim 3 \times 10^6$...

D I: 10.1103/ ... B87.275508 AC ... : 61.72. , 61.43. , 71.15. , 71.23. R

VE ... 1- ...

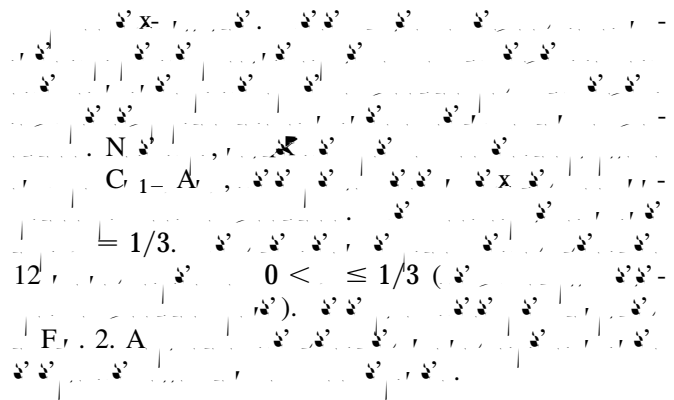
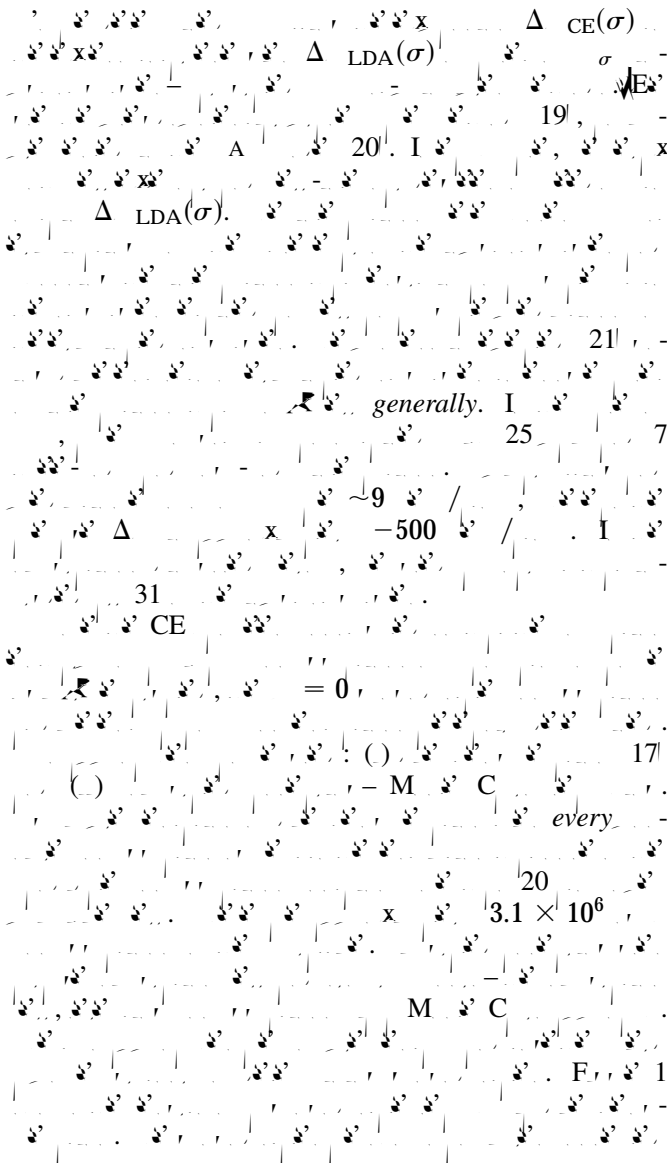


FIG. 1. Evolution of the LDA-CE system for $\sigma \sim 3 \times 10^6$ (circles) and $\sigma \sim 10^6$ (squares). The panels are labeled 1 through 12. The y-axis is labeled 'Energy' and the x-axis is labeled 'Number of particles'.

$x = 8, 23$.
Long range order.
 $(F, 2) : ()$
 $(111) : ()$
 $(111) : (112)$
 $F x = 1/6$
 $1 \ 2 \ 1 \ 8 \ ()$

