

Please show calculations on additional sheets. Use a straightedge to neatly plot additional peaks.

1) The electron density $\rho(x)$ for a 1-D crystal containing two point-like atoms is shown on the left:

An atom of type A is at $x_A = 0.0$. An atom of type B is at $x_{B1} = 0.9$.

(Note the relative heights of A and B.)

Label the areas of the peaks in the graph for $P(x)$ (left).

2) Next, an atom of type B is added to the crystal. $P(x)$ for this structure is shown (bottom right).

a) Determine the location of the second B atom (x_{B2})

b) Complete the graph for $\rho(x)$, by showing the peak for the second B atom, with the label “B”.

c) Label the areas of all peaks in $P(x)$

