

Date:

Name:

Q: Show that *i*) if a wavefunction  $\psi$  is described by a Bloch state, its square modulus contributing to the charge density is periodic; *ii*) if  $\psi$  is expanded in plane-waves up to a given kinetic energy cutoff  $E_{cutwfc}$ , show that the charge density has non zero Fourier components up to  $4 \times E_{cutwfc}$ . Moreover, show that *iii*) if Fourier components of  $V(r) \cdot \psi(r)$  are desired only up to  $E_{cutwfc}$ , Fourier components of  $V(r)$  only up to  $4 \times E_{cutrho}$  are needed.

A:

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Indicate here a possible topic you would like to be covered during this course or a subject that you would like to be clarified further (we'll see what can be done, but no commitment):

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