Electronic polarization in quasilinear chains MICHAEL SPRING-
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bruecken, Germany — Starting with a finite k-mesh version of a well-known equation
of Blount, we show how various definitions proposed for the polarization of a long
chain are related. Expressions used for infinite periodic chains in the 'modern theory
of polarization' are thereby obtained along with a new single-particle formulation.
Separate intracellular and intercellular contributions to the polarization are identi-
fied and in application to infinite chains, the traditional sawtooth definition is found
to be missing the latter. For a finite open chain the dipole moment depends upon
how the chain is terminated, but the intracellular and intercellular polarization do
not. All these results are illustrated through calculations with a simple Hückel-like
model.

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