



Band structure of the one dimensional metallic (SN) x crystal

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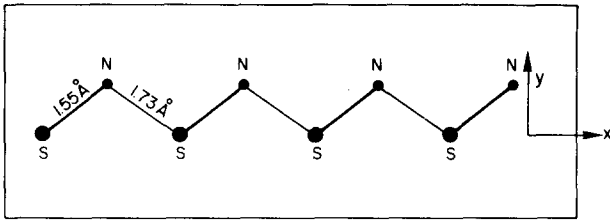


FIG. 1. Crystal structure of a one-dimensional alternant (SN)_x crystal.

the one-dimensional group character, one can display these bands in the primitive Brillouin zone (one molecule per cell) without loss of information.] Bloch functions $\Phi_\mu^\alpha(\mathbf{K}, \mathbf{r})$ for the α sublattice and the μ th atomic orbital $\chi_\mu(\mathbf{r}-\mathbf{R}_n-\mathbf{d}_\alpha)$ are constructed as

$$\Phi_\mu^\alpha(\mathbf{K}, \mathbf{r}) = N^{-1/2} \sum_{n=1}^N e^{i\mathbf{K} \cdot \mathbf{R}_n} \chi_\mu(\mathbf{r} - \mathbf{R}_n - \mathbf{d}_\alpha), \quad (1)$$

where \mathbf{R}_n denotes the position of unit cell n , \mathbf{d}_α denotes the coordinates of the internal position of the atom, belonging to sublattice α ($\alpha = 1, 2, \dots, h$ for the diatomic molecules, $h = 2h'$), and N indicates the number of unit

$$- \sum_a \sum_m \frac{Z_a}{\mathbf{r}_1 - \mathbf{d}_a - \mathbf{R}_m} |\chi_\nu(\mathbf{r}_1 - \mathbf{R}_n - \mathbf{d}_\beta)\rangle, \quad (6)$$

and Z_a denotes the core-charge of atom a . $(\mu n, \gamma m | \mu' s \lambda' t)$ denotes the two-electron term

$$(\mu n, \lambda m | \mu' s, \lambda' t) = \langle \chi_\mu(\mathbf{r}_1 - \mathbf{R}_n) \chi_\lambda(\mathbf{r}_1 - \mathbf{R}_m) | \frac{1}{\mathbf{r}_{12}} | \chi_{\mu'}(\mathbf{r}_2 - \mathbf{R}_s) \chi_{\lambda'}(\mathbf{r}_2 - \mathbf{R}_t) \rangle \quad (7)$$

and $P_{\mu'\nu',st}^{\alpha,\beta}$ is the integral over the occupied part of the Brillouin zone (BZ) of the wave vector dependent bond-charge density matrix $P_{\mu'\nu',st}^{\alpha,\beta}(\mathbf{K})$:

$$P_{\mu'\nu',st}^{\alpha,\beta} = \int_{\text{BZ}_{oc}} d^3\mathbf{K} P_{\mu'\nu'}^{\alpha,\beta}(\mathbf{K}) e^{i\mathbf{K}(\mathbf{R}_s - \mathbf{R}_t)} = P_{\mu'\nu',st}^{\alpha,\beta}(s-t), \quad (8)$$

where the notation of the BZ_{oc} integration volume implies an integration over the first BZ for the fully occupied bands and up to the Fermi momentum \mathbf{K}_F for partially occupied bands. The wave vector dependent bond-charge matrix has elements given by

$$P_{\mu'\nu',st}^{\alpha,\beta}(\mathbf{K}) = \sum_j^{a_{oc}} n_j [C_{\mu',j}^{\alpha}(\mathbf{K})]^* [C_{\nu',j}^{\beta}(\mathbf{K})]; \quad (9)$$

