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

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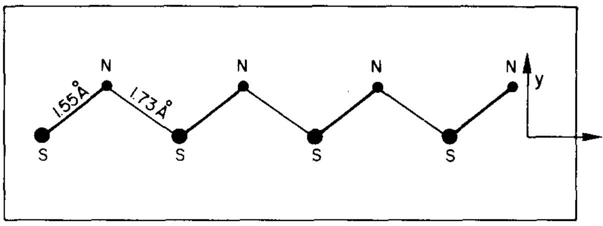

FIG. 1. Crystal structure of a one-dimensional alternant (SN)$_x$ crystal.

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 $\alpha$ sublattice and the $\mu$th atomic orbital $\chi_\mu(\mathbf{r}-\mathbf{R}_n-\mathbf{d}_\alpha)$ are constructed as

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

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

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

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

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

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 $P_{\mu',\nu'}^{\alpha,\beta}(\mathbf{K})$:

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

where the notation of the $\mathrm{BZ}_{oc}$ 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

$$P_{\mu',\nu'}^{\alpha;\beta}(\mathbf{K}) = \sum_j^{\sigma_{oc}} n_j \left[C_{\mu',j}^\alpha(\mathbf{K})\right]^* \left[C_{\nu',j}^\beta(\mathbf{K})\right]; \tag{9}$$