

## LIST OF SYMBOLS – CHAPTER A

$R$	group symmetry operation
$\mathbf{R}$	double group symmetry operation
$\psi_i$	basis function
$\Gamma(R)_{ij}^{(n)}$	group representation matrix element
$\rho_{ij}^{(n)}$	group projection operator
$X(R)$	trace of representation, character
$\varphi_k$	class of group symmetry operations
$f(\mathbf{r})$	function
$E$	energy
$H$	Hamiltonian
$\mathbf{t}, \boldsymbol{\tau}$	real space vector
$\mathbf{a}_i$	lattice basis vector
$\alpha$	rotational part of group symmetry operation
$\varepsilon$	identity
$\mathbf{L}$	lattice vector
$\mathbf{b}_i$	reciprocal basis vector
$\mathbf{G}, \mathbf{k}$	vector in reciprocal space
$G$	space group
$\mathbf{D}$	double space group
$G^0$	point group
$T$	translation group
$G/T$	factor group
$G_{\mathbf{k}}$	‘small’ space group
$G_{\mathbf{k}}^0$	‘small’ point group
$G_{\mathbf{k}}/T_{\mathbf{k}}$	‘small’ factor group
$\theta, \phi, \psi$	Eulerian angles
$D_{1/2}$	spin representation matrices
$u_s$	spin function
$\boldsymbol{\sigma}$	spin operator
$T$	time reversal operator
$U$	unitary operator
$K$	complex conjugation operator

## LIST OF SYMBOLS – CHAPTER B

$H$	Hamiltonian
$\left. \begin{array}{l} \psi_{nk}(\mathbf{r}) \\ \phi_{nk}(\mathbf{r}) \\ \Phi_{nk}(\mathbf{r}) \end{array} \right\}$	Bloch functions
$\varphi(\mathbf{r})$	Atomic Löwdin function
$\hbar$	Planck's constant
$m$	effective electron mass
$\nabla$	gradient operator
$V(\mathbf{r})$	one electron potential
$\mathbf{r}, \mathbf{R}_l, \boldsymbol{\tau}_\alpha, \mathbf{Q}, \mathbf{d}$	real space vectors
$\mathbf{k}, \mathbf{G}$	reciprocal space vectors
$X_j(\mathbf{r})$	atomic orbital
$R_{\alpha j}(r), u_{\alpha j}(r)$	radial wave function
$\rho(\mathbf{r})$	electron density
$S, L$	transformation matrices
$j_l(kr)$	spherical Bessel function
$Y_{lm}(\theta, \phi)$	spherical harmonic
$\theta, \phi$	polar angles
$ c\rangle$	core state
$ \mathbf{k}\rangle$	plane wave state
$S_\beta(\mathbf{G})$	structure factor
$V_{\beta L}(\mathbf{G})$	form factor
$\boldsymbol{\sigma}$	spin Pauli matrices
$\mathbf{P}_l$	angular projection operator
$P_l$	Legendre polynomial of order $l$
$P_c$	core states projection operator
$G_{\mathbf{k}}(\mathbf{r}, \mathbf{r}')$	Green's function
$n_l(kr)$	spherical Neumann function
$U_j^{(l)}$	free electron wave function
$Q$	transfer matrix
$H_l^{(1)}$	Hankel function of first kind
$\zeta$	complex variable
$J_{ M }$	Bessel function

## LIST OF SYMBOLS – CHAPTER C

$V(q)$	potential Fourier transform form factor
$S(q)$	structure factor
$\epsilon(q)$	static dielectric function (real part)
$\epsilon_1(\omega)$	real part of dielectric function
$\epsilon_2(\omega)$	imaginary part of dielectric function
$\hbar$	Planck's constant
$E$	energy
$\omega$	light frequency
$\nabla$	gradient operator
$U_{\alpha\mathbf{k}}$	periodic part of Bloch function
$\rho(\mathbf{r})$	charge density
$\mathbf{R}_m$	lattice vector
$\mathbf{k}$	reciprocal space vector
$N(E)$	density of states
$\mu$	reduced mass
$\mathbf{A}$	vector potential
$a(\mathbf{r})$	Wannier function
$\alpha$	anisotropy parameter