Site Symmetry in crystals : basis of the theory and applications for the electron and phonon states.

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Site Symmetry in Crystals

Theory and Applications

Second Enlarged Edition



R. A. Evarestov Quantum Chemistry of Solids The LCAO

First Principles Treatment of Crystals



Site symmetry approach establishes symmetry relations between the localized states (atomic electron states and atomic displacements) and extended molecular or crystalline states (symmetry of molecular or crystalline orbitals and phonons). The localized states transform according to the irreducible representations (irreps) of the site symmetry point groups (in crystalspoint symmetry groups of Wyckoff positions occupied by atoms). The extended states transform according to the irreps of the space group of the crystal (point group of the molecule). The extended states are induced from the localized states.



Fig. 3.8. MnO_4^- ion

KMnO₄ Pnma (62- D_{2h}^{16}) Z=4 4c .m. x 0.25 z 8d 1 x y z K, Mn –4c O-4c,4c,8d (**MnO₄**)⁻ Mn-T_d O-C_{3v}

Point Group Tables of T_d(-43m)

Character Table

T _d (-43m)	#	E	3	2	-4	m	functions
Mult.	-	1	8	3	6	6	
A ₁	Г1	1	1	1	1	1	x ^{2+y2+z²}
A ₂	Γ2	1	1	1	-1	-1	
E	Гз	2	-1	2	0	0	(2z ² -x ² -y ² ,x ² -y ²)
T ₁	Г4	3	0	-1	1	-1	$(J_{\mathbf{X}},J_{\mathbf{Y}},J_{\mathbf{Z}})$
T ₂	Г5	3	0	-1	-1	1	(x,y,z),(xy,xz,yz)

Point Group Tables of C_{3v}(3m)

Character Table

C _{3v} (3m)	#	1	3	m	functions
Mult.	-	1	2	3	
A ₁	Γ ₁	1	1	1	z,x ²⁺ y ² ,z ²
A ₂	Г2	1	1	-1	Jz
E	Г3	2	-1	0	$(x,y),(xz,yz),(x^2-y^2,xy),(J_x,J_y)$

 $G=T_d=H_{Mn}$ $H_O=C_{3v}$

Subduced in (correlation	reps of T _o table)	a Indi	uced irreps of T _d
	T _d a ₁ a ₂ e t ₁ t ₂ (x,y,z)	C _{3v} a ₁ a ₂ e a ₂ e a ₁ e	$\begin{array}{cccc} C_{_{3v}} & T_{_{d}} \\ a_{_{1}}(z) & a_{_{1}}t_{_{2}} \\ a_{_{2}} & a_{_{2}}t_{_{1}} \\ e & (x,y) & e t_{_{1}}t_{_{2}} \end{array}$

The Frobenius reciprocity theorem is proved [13]: the multiplicity of an irrep $D^{(\alpha)}(g)$ of G in a rep $d^{[\gamma]} \uparrow G$ induced by an irrep $d^{(\gamma)}$ of $H \subset G$ is equal to the multiplicity of an irrep $d^{(\gamma)}$ of H in the rep $D^{(\alpha)} \downarrow H$ subduced by $D^{(\alpha)}$ of H.





Perovskite $CaTiO_3$ Ca 1b (0.5, 0.5, 0.5) Ti 1a (0,0,0) 0 3d (0.5, 0, 0; 0,0.5,0; 0, 0, 0.5) (abd)= (bac) Z=1, Pm-3m(221- O_h^1)

Anatase TiO₂

two Ti atoms 2a(0, 0, 0; 0, 1/2, 1/4), four oxygen atoms 4e(0, 0, u; 1/2, 0, -u + 1/2; 0, 1/2, u + 1/4; 1/2, 1/2, -u + 1/2). The anatase structure is defined by three parameters: a, c, u. (a e) = (b e) $Z = 2, I4_1/amd$

141-D_{4h}¹⁹

Brillouin Zones

Simple cubic lattice Tetragonal bc lattice



3X(0.5 0 0) 3M(0.5 0.5 0)



Γ (000) M (0.5 0.5 0.5) 2P(0.25 0.25 0.25) 2X (0 0 0.5) 4N (0 0.5 0)

SYMMETRY OF LOCALIZED STATES IN PEROVSKITE AND ANATASE

Perovskite CaTiO₃

 $\begin{array}{ccccc} Ti & a & s & a_{1g} \\ & Oh & (x,y,z) & t_{1u} \\ Ca & b & (z^2,x^2\!\!\cdot\!y^2) & e_g \\ & & & (xy,xz,yz) & t_{2g} \end{array}$

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	T _{tu}	۲ <mark>4</mark>	3	1	-1	0	-1	-3	-1	1	0	1	(x,y,z)		
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	a_{1u}	1^{-}	1^{-}	2+	1-	4-	1-	3+
	a_{2g}	2+	2+	1^{-}	2+	3+	2+	4-
a	a_{2u}	2^{-}	2^{-}	1+	2-	3-	2-	4+
	e_g	3^{+}	3+	3-	$1^{+}2^{+}$	$3^{+}4^{+}$	$1^{+}2^{+}$	$3^{-}4^{-}$
b	e_u	3-	3-	3+	$1^{-2^{-}}$	3-4-	$1^{-2^{-}}$	$3^{+}4^{+}$
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	t_{1u}	4-	4-	5^{+}	$3^{-5^{-}}$	$2^{-5^{-}}$	$3^{-5^{-}}$	$1^{+}5^{+}$
	t_{2g}	5^{+}	5+	4-	$4^{+}5^{+}$	$1^{+}5^{+}$	$4^{+}5^{+}$	$2^{-5^{-}}$
	t_{2u}	10	5-	4+	$4^{-5^{-}}$	$1^{-5^{-}}$	$4^{-5^{-}}$	$2^{+}5^{+}$
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	a_{1g}	$1^{+}3^{+}$	5+	4-	4+5-	$1^{+}5^{-}$	$1^{+}3^{-}4^{-}$	$1^{+}2^{+}3^{-}$
	a_{1u}	$1^{-}3^{-}$	5-	4+	$4^{-5^{+}}$	$1^{-5^{+}}$	$1^{-}3^{+}4^{+}$	$1^{-}2^{-}3^{+}$
	b_{2g}	$2^{+}3^{+}$	4+	5^{-}	$3^{+}5^{-}$	$2^{+}5^{-}$	$2^{+}3^{-}4^{-}$	$1^{+}2^{+}4^{-}$
c	b_{2u}	$2^{-}3^{-}$	4-	5^{+}	$3^{-5^{+}}$	$2^{-5^{+}}$	$2^{-}3^{+}4^{+}$	$1^{-}2^{-}4^{+}$
	a_{2g}	4+	$2^{+}3^{+}$	$1^{-}3^{-}$	$2^{+}3^{-}4^{-}$	$1^{-}2^{-}3^{+}$	$3^{+}5^{-}$	$1^{-5^{+}}$
d	a_{2u}	4-	$2^{-3^{-}}$	$1^{+}3^{+}$	$2^{-}3^{+}4^{+}$	$1^{+}2^{+}3^{-}$	$3^{-5^{+}}$	$1^{+}5^{-}$
	b_{1g}	5+	$1^{+}3^{+}$	$2^{-}3^{-}$	$1^{+}3^{-}4^{-}$	$1^{-}2^{-}4^{+}$	$4^{+}5^{-}$	$2^{-5^{+}}$
	b_{1u}	5-	$1^{-3^{-}}$	$2^{+}3^{+}$	$1^{-3+4^{+}}$	$1^{+}2^{+}4^{-}$	$4^{-5^{+}}$	$2^{+}5^{-}$
	e_g	$4^{+}5^{+}$	$4^{+}5^{+}$	$4^{-}5^{-}$	$1^{-}2^{-}5^{+}5^{-}$	$3^{-}4^{-}5^{+}5^{-}$	$1^{-}2^{-}5^{+}5^{-}$	$3^+4^+5^+5^-$
	e_u	$4^{-}5^{-}$	$4^{-5^{-}}$	$4^{+}5^{+}$	$1^{+}2^{+}5^{-}5^{+}$	$3^+4^+5^-5^+$	$1^+2^+5^-5^+$	$3^{-}4^{-}5^{-}5^{+}$

Table 3.8. Simple induced representations of the O_h^1 - $Pm\overline{3}m$ space group

In (aaa) units: $a_1(100)$, $a_2(010)$, $a_3(001)$ $Q: O_h(m\overline{3}m) - a(000)$, b(1/2, 1/2, 1/2); $D_{4h}(4/mmm) - c(1/2, 1/2, 0)$, d(1/2, 0, 0)In $(2\pi/a, 2\pi/a, 2\pi/a)$ units: $b_1(100)$, $b_2(010)$, $b_3(001)$ $K: O_h - \Gamma(000)$, R(1/2, 1/2, 1/2); $D_{4h} - M(1/2, 1/2, 0)$, X(1/2, 0, 0)

Induced site-symmetry representations of space group: P m -3 m (221)

with K-vector: G=(0, 0, 0)

[Symmetry elements Space Group P m -3 m (221)]

WP	Representative
1a	0.0.0

Site Symmetry Group

Site Symmetry Group for 0,0,0 (1a)

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G(1) a_{1g} 1⁺ ;G(2) a_{1u} 1⁻; G(3) a_{2g} 2⁺; G(4) a_{2u} 2⁻; G(5) e_{u} 3⁻; G(6) e_{g} 3⁺; G(7) t_{2u} 5⁻; G(8) t_{2g} 5⁺; G(9) t_{1u} 4⁻; G(10) t_{2u} 4⁺

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s, z² x²-y² a D_{2d} Ti z, xy (x, y), (xz, yz)



 a_1 b_1

 b_2

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	C_{2} (mm2)	#	1	2 _z	my	$\mathbf{m}_{\mathbf{x}}$	functions					
	A ₁	Γ ₁	1	1	1	1	z,x²,y²,z²					
	A ₂	Гз	1	1	-1	-1	xy,J _z					
	B ₁	Γ ₂	1	-1	1	-1	x,xz,J _y					
	B ₂	Г4	1	-1	-1	1	y,yz,J _x					

[List of imeducible representations in matrix form]

q	β	Г	М	X		Р	N	
					а	b		
a	a,	1+4-	1	1	2	1	1+2-	
	a2	3+2-	2	2	2	1	1-2*	
b	b2	3-2+	1	2	1	2	1+2-	
	b,	1-4+	2	1	1	2	1-2+	
	e	5+5-	34	12	1 2 1 2		1+1-2+2-	
							с	d
с	a	1*2*5*	14	1 2	1 2		1+1+2+2-	1+1-2-2-
	a,	1-2-5-	24	1 2	1 2		1-1-2+2-	1*1-2+2+
d	b.	3*4*5*	2 3	12	1 2		1+1-2+2+	1-1-2+2-
	b.	3-4-5-	1 3	12	1	2	1+1-2-2-	1*1*2*2-

Table 4.21. Simple induced representations of the $D_{4b}^{19} - I4_1/amd$ space group

The basis translations vectors of direct and reciprocal lattices and coordinates of K-set points are in Table 4.20.

$$Q: D_{2d}(\bar{4}m2) - a(000), b(1/2, 1/2, 0); \\ C_{2h}(.2/m.) - c(3/8, 1/8, 1/4), d(-1/8, -3/8, 1/4)$$



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Induced site-symmetry representations of space group: I 4,/a m	d				
(141)					
with K-vector: N=(0, 0, 5, 0)					
[Summetry elements Space Group L4 /a m d (141)]		Induced representations			
	Induced representations for the point N of I 4 ₁ /a m d				
WP Representative					
4a 0,3/4,1/8		Irreps)Reps (*N)(1) (*N)(2) (*N)(3) (*N)(4)			
Site Symmetry Group					
Site Symmetry Group for 0,3/4,1/8 (4a)					
		A ₂ 1 · 1			
$\begin{bmatrix} y_1 \\ x,y,z \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0$	-	B_1 1 · · 1			
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N(1) Site Synmetry 1; N(3) 2*; N(4) 2-	ũ-	E 1 1 1 1			
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Irreducible representations					
Character table for -42m					
D_{2d} (-42m) # 1 2 -4 2_x m_d functions					
Mult 1 1 2 2 2 ·					
A_4 Γ_4 1 1 1 1 1 $V_{x^2+v^2-7^2}$					
		N(1) 1 ⁺ ; N(2) 1 ⁻ ; N(3) 2 ⁺ ; N(4) 2 ⁻			
A_2 I_2 I_1 I_1 I_2 I_1 I_2 I_3 I_2					
$\begin{bmatrix} B_{1} & F_{3} \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ x^{2} - y^{2} \end{bmatrix}$					
B ₂ Γ ₄ 1 1 -1 -1 1 z,xy					
Subduced representations					
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N(1) 1⁺; N(2) 1⁻; N(3) 2⁺; N(4) 2⁻

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C _{2v} (mm2)	#	1	2 _z	m _y	m _x	functions
A ₁	Γ ₁	1	1	1	1	z,x²,y²,z²
A ₂	Γ ₃	1	1	-1	-1	xy,J _z
B ₁	Γ ₂	1	-1	1	-1	x,xz,J _y
B ₂	Γ ₄	1	-1	-1	1	y,yz,J _x

Subduced representations

Character table for the subduced representations (*N4mm2) for Wyckoff

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THANKS FOR ATTENTION!