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Local electronic states of Fe^{2+} ions in orthopyroxene

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Appendix A: Spin-orbit coupling matix with the basis $\{\chi_k(M_s)\}$ [a]

	$\chi_1(2)$	$\chi_1(1)$	$\chi_1(0)$	$\chi_1(-1)$	$\chi_1(-2)$	$\chi_2(2)$	$\chi_2(1)$	$\chi_2(0)$	$\chi_2(-1)$	$\chi_2(-2)$	$\chi_3(2)$	$\chi_3(1)$	$\chi_3(0)$	$\chi_3(-1)$	$\chi_3(-2)$
$\chi_1(2)$						$4\lambda S$						λY_+			
$\chi_1(1)$							$2\lambda S$				λY_+		$\frac{\sqrt{6}}{2}\lambda Y_+$		
$\chi_1(0)$												$\frac{\sqrt{6}}{2}\lambda Y_+$		$\frac{\sqrt{6}}{2}\lambda Y_+$	
$\chi_1(-1)$									$-2\lambda S$				$\frac{\sqrt{6}}{2}\lambda Y_+$		λY_+
$\chi_1(-2)$										$-4\lambda S$				λY_+	
$\chi_2(2)$	$4\lambda S$											$-\lambda$			
$\chi_2(1)$		$2\lambda S$									λ		$-\frac{\sqrt{6}}{2}\lambda$		
$\chi_2(0)$												$\frac{\sqrt{6}}{2}\lambda$		$-\frac{\sqrt{6}}{2}\lambda$	
$\chi_2(-1)$				$-2\lambda S$									$\frac{\sqrt{6}}{2}\lambda$		$-\lambda$
$\chi_2(-2)$					$-4\lambda S$									λ	
$\chi_3(2)$		λY_+					λ								
$\chi_3(1)$	λY_+		$\frac{\sqrt{6}}{2}\lambda Y_+$			$-\lambda$		$\frac{\sqrt{6}}{2}\lambda$							
$\chi_3(0)$		$\frac{\sqrt{6}}{2}\lambda Y_+$		$\frac{\sqrt{6}}{2}\lambda Y_+$			$-\frac{\sqrt{6}}{2}\lambda$		$\frac{\sqrt{6}}{2}\lambda$						
$\chi_3(-1)$			$\frac{\sqrt{6}}{2}\lambda Y_+$		λY_+			$-\frac{\sqrt{6}}{2}\lambda$		λ					
$\chi_3(-2)$				λY_+					λ						

a. $s = \sin x$, $c = \cos x$, $Y_+ = \sqrt{3}\cos x + \sin x$, $\lambda = -\zeta_d/4$, and $\zeta_d = \int_0^\infty R_{3d}^{\,2}(r)\,\xi(r)\,r^2 dr$, $R_{3d}(r)$ being the radial wavefunction of the Fe^{2+} ion.

Appendix B: Matrices of the electron EFG operators $V_{\alpha\beta}^{val}$ with the basis $\{\chi_k(M_S)\}$ $(k = 1, 2, 3;\ M_S = 0, \pm 1, \pm 2)$[a,b]

$V_{xx}^{val}/e\langle r^{-3}\rangle$	$\chi_1(M_S)$	$\chi_2(M_S)$	$\chi_3(M_S)$
$\chi_1(M_S)$	$2z_+/7$		
$\chi_2(M_S)$		$-2/7$	
$\chi_3(M_S)$			$4/7$

$V_{yy}^{val}/e\langle r^{-3}\rangle$	$\chi_1(M_S)$	$\chi_2(M_S)$	$\chi_3(M_S)$
$\chi_1(M_S)$	$-2z_-/7$		
$\chi_2(M_S)$		$-2/7$	
$\chi_3(M_S)$			$-2/7$

$V_{zz}^{val}/e\langle r^{-3}\rangle$	$\chi_1(M_S)$	$\chi_2(M_S)$	$\chi_3(M_S)$
$\chi_1(M_S)$	$-4c_2/7$		
$\chi_2(M_S)$		$4/7$	
$\chi_3(M_S)$			$-2/7$

$V_{xy}^{val}/e\langle r^{-3}\rangle$	$\chi_1(M_S)$	$\chi_2(M_S)$	$\chi_3(M_S)$
$\chi_1(M_S)$		$2\sqrt{3}c/7$	
$\chi_2(M_S)$	$2\sqrt{3}c/7$		
$\chi_3(M_S)$			

$V_{yz}^{val}/e\langle r^{-3}\rangle$	$\chi_1(M_S)$	$\chi_2(M_S)$	$\chi_3(M_S)$
$\chi_1(M_S)$			$\sqrt{3}y_-/7$
$\chi_2(M_S)$			
$\chi_3(M_S)$	$\sqrt{3}y_-/7$		

$V_{zx}^{val}/e\langle r^{-3}\rangle$	$\chi_1(M_S)$	$\chi_2(M_S)$	$\chi_3(M_S)$
$\chi_1(M_S)$			
$\chi_2(M_S)$			$-3/7$
$\chi_3(M_S)$		$-3/7$	

a. $s = \sin x$, $c = \cos x$, $s_2 = \sin(2x)$, $c_2 = \cos(2x)$, $y_- = \sqrt{3}s - c$, $z_+ = \sqrt{3}s_2 + c_2$, $z_- = \sqrt{3}s_2 - c_2$.

b. Since EFG operators do not contain spin, it is easy to prove that

$$\langle \chi_i(M_S)|\, V_{\alpha\beta}^{val} |\chi_j(M_S')\rangle = \langle \chi_i(M_S)|\, V_{\alpha\beta}^{val} |\chi_j(M_S)\rangle \delta_{M_S M_S'}\ , \text{ and}$$

$$\langle \chi_i(M_S)|\, V_{\alpha\beta}^{val} |\chi_j(M_S)\rangle = \langle \chi_i(M_S')|\, V_{\alpha\beta}^{val} |\chi_j(M_S')\rangle\ .$$