	MAEsc	$D_{B, d_{z^2}}^{\uparrow +}$	$q_B$	$E_{B, d_{xy}}^{\downarrow -}$	$E_{B,d_{x^2-y^2}}^{\uparrow-}$	$E_{B,d_{xy}}^{\uparrow}$	$D_{B, d_{x^2-y^2}}^{\uparrow -}$	$I_{B,d_{z^2}}^{\downarrow+}$	$E_{B, d_{x^2-y^2}}^{\downarrow -}$	$D_{B, d_{x^2-y^2}}^{\downarrow -}$	$D_{T, d_{z^2}}^{\uparrow +}$	$E_{T,d_{Z^2}}^{\uparrow+}$	$D_{B,d_{z^2}}^{\downarrow+}$	$DOS_{T, d_{z^2}}^{\downarrow}$	BG ↓	$\int_{T, d_{xz}}^{\uparrow}$	$D_{B,d_{xy}}^{\uparrow}$	$DOS_{B, d_{Z^2}}^{\downarrow}$	$D_{B,d_{xz}}^{\downarrow+}$	$I_{B, d_{xy}}^{\downarrow -}$	$D_{T, d_{yz}}^{\uparrow +}$		1.00
MAE <sub>SC</sub> -		-0.33	-0.33	-0.30	-0.29	-0.29	-0.26	0.24	-0.24	-0.22	-0.21	0.21	0.20	-0.20	0.20	-0.19	-0.19	-0.18	-0.18	-0.18	-0.18		- 1.00
$D_{B,d_{z^2}}^{\uparrow+}$			0.37	0.24	0.30	0.30	0.30	-0.17	0.18	0.30	0.35	-0.19	-0.11		-0.15		0.33				0.26		
$q_B$ -				0.20	0.31	0.32	0.27	-0.13	0.16	0.25	0.31	-0.37		-0.11		0.18	0.26	-0.13			0.35	-	- 0.75
$E_{B,d_{xy}}^{\downarrow -}$		-	•		0.47	0.54	0.32	-0.20	0.59	0.31	0.11		-0.20	0.19	-0.18		0.29	0.17	0.20	0.37			
$E_{B,d_{x^2-y^2}}^{\uparrow -}$		•				0.49	0.30	-0.26	0.53	0.22	0.10		-0.24	0.18	-0.16		0.32	0.16		0.23			
$E_{B,d_{xy}}^{\uparrow-}$			•		•		0.28	-0.23	0.47	0.26	0.14	-0.16	-0.20	0.14	-0.13		0.26	0.13		0.29	0.12		- 0.50
$D_{B, d_{x^2-y^2}}^{\uparrow -}$						-			0.25	0.54							0.48		0.26				
$I_{B, d_{z^2}}^{\downarrow +} -$		-	•	•	•	-			-0.19		-0.15		0.56	-0.28	0.21	-0.22		-0.27	-0.11	-0.24	-0.14		- 0.25
$E_{B,d_{x^2-y^2}}^{\downarrow -}$		-	•			•		-		0.17			-0.19	0.19	-0.17		0.23	0.19	0.12	0.35			
$D_{B, d_{x^2-y^2}}^{\downarrow -}$		•	•	•	•	-	•		•		0.14						0.43		0.31				
$D_{T,d_{z^2}}^{\uparrow+}$		•	•	•	•	=		-		=		-0.38	-0.10			0.31					0.29		- 0.00
$E_{T,d_{z^2}}^{\uparrow+}$		-	•			-										-0.24					-0.29		
$D_{B, d_{z^2}}^{\downarrow +}$ -		-		-	-	-			-		•			-0.36	0.15	-0.21		-0.37		-0.22	-0.14		0.25
$DOS_{T, d_{z^2}}^{\downarrow}$	•		-	-	-	-		-	-				•		-0.39	0.14		0.70	0.11	0.36			0.25
BG <sub>dir</sub> -		-		-	_	-		-	-				-	•				-0.47	-0.16	-0.34			
$I_{T, d_{xz}}^{\uparrow, -}$			•					-				•	•	•				0.16		0.13	0.21		0.50
$D_{B, d_{xy}}^{\uparrow -}$	•	•		•	•	-	•		•										0.16				
$DOS_{B, d_{z^2}}^{\downarrow}$	•		-		-	-		-	-				•		-	-				0.37			
$D_{B, d_{xz}}^{\downarrow +}$				•			•	•	•	•				•	•		•			0.14			0.75
$I_{B, d_{xy}}^{\downarrow -}$					•	•		•					•		•				•				
$D_{T,d_{yz}}^{\uparrow}$	-			-		-		-				•	-										1.00