substance: CoO
property: band structure, energy gap, interband transition energies

band structure: Fig. 1 (see also [72M1, 78K]).

energy gaps

E_g	2.6 eV	RT	absorption: Fig. 2; fundamental edge shifts to higher energy at lower temperature. Below 290 K, sample showed optical anisotropy.	59P, 70P
$E_{g,th}$	3.6(5) eV		from Hall data in Ti doped CoO	72G

width of bands

W(O 2p band)	≈ 4 eV	RT	XPE spectra, (core region, see Fig. 3)	79J,
W(Co 3d band)	< 3 eV	RT		75K

higher transition energies from optical spectra

E_{peak}	5.5(5.7) eV	RT	absorption (Fig. 4). Value in	70P
	7.5 eV	(shoulder	parentheses from [72M2].	
	12.6 eV	at 8.5 eV found		
	17.5 eV	at 120 K)		
			thermoreflectance (Fig. 5), assignment of final state (cf. Fig. 6)	72M2
	2.8 eV	RT	I: $d^6(t_\alpha^3 t_\beta e_\alpha^2) + 4s$	
	3.2 eV	RT	II: $d^6(t_\alpha^3 t_\beta e_\alpha^2) + d^8(t_\alpha^3 t_\beta^2 e_\alpha^2)$	
	3.8 eV	RT	III: $d^6(t_\alpha^3 t_\beta^2 e_\alpha) + 4s$	
	4.2 eV	T = 80 K	IV: $d^6(t_\alpha^3 t_\beta e_\alpha^2) + d^8(t_\alpha^3 t_\beta^2 e_\alpha^2 e_\beta)$ and $d^6(t_\alpha^3 t_\beta^2 e_\alpha) + d^8(t_\alpha^3 t_\beta^3 e_\alpha^2)$	
	4.75 eV	RT	V: $d^6(t_\alpha^2 t_\beta^2 e_\alpha^2) + 4s$	
	5.0 eV	T = 80 K	V: $d^6(t_\alpha^2 t_\beta^2 e_\alpha^2) + 4s$	
	5.35 eV	T = 80 K	VI: $d^6(t_\alpha^3 t_\beta^2 e_\alpha) + d^8(t_\alpha^3 t_\beta^2 e_\alpha^2 e_\beta)$	
	5.75 eV	RT	O 2p – Co 4s (onset)	
	6.0 eV	T = 80 K	O 2p – Co 4s (onset)	
	6.25 eV	T = 80 K	VII: $d^6(t_\alpha^2 t_\beta^2 e_\alpha^2) + d^8(t_\alpha^3 t_\beta^2 e_\alpha^2 e_\beta)$	
	7.2 eV	T = 80 K	O 2p – Co 4s	
	7.0 eV	RT	O 2p – Co 4s	
			empirical energy level scheme, Fig. 6.	
		RT	EELS, radically different assignment:	76A
	2.2 eV		not assigned	
	3.3 eV		O 2p – Co t_β	
	4.6 eV		O 2p – Co t_β	
	5.6 eV		O 2p – Co e_β	
	6.8 eV		O 2p – Co e_β	
	7.6 eV		O 2p – Co 4s	
	9.7 eV		O 2p – Co 4s	

References:

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Fig. 1.

CoO. (a) Hartree-Fock, (b) self-consistent calculation with correlation, (c) non-self consistent calculation of the band structure, (d) experimental photoemission spectrum of [75E]. [78K].

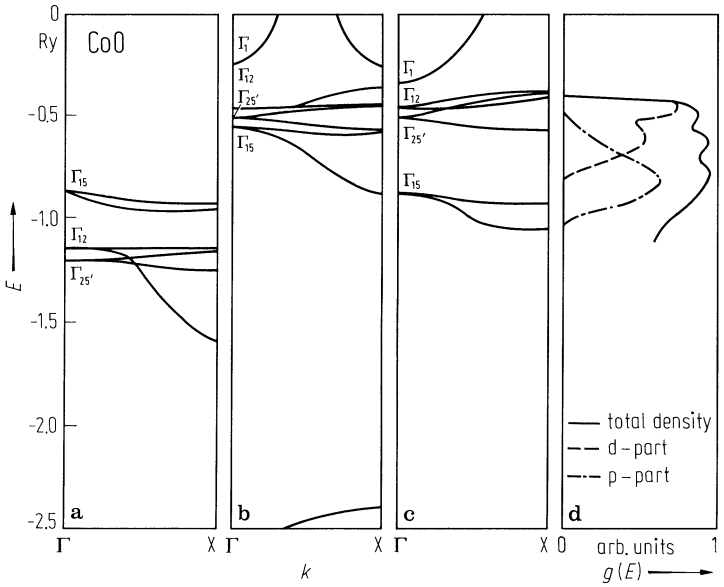

Fig. 2.

CoO. Absorption coefficient vs. wavelength (photon energy) at 80 K and 298 K. Unpolarized light, sample (100) plane [59P].

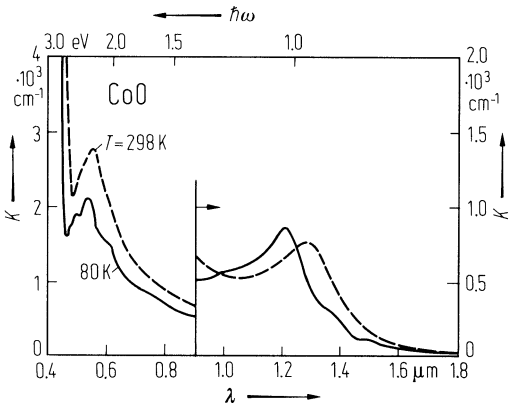

Fig. 3.

CoO. XPS spectrum in the core region (intensity vs. binding energy) [75K]. For assignment of various peaks, see original paper. E_b: binding energy relative to the Fermi level.

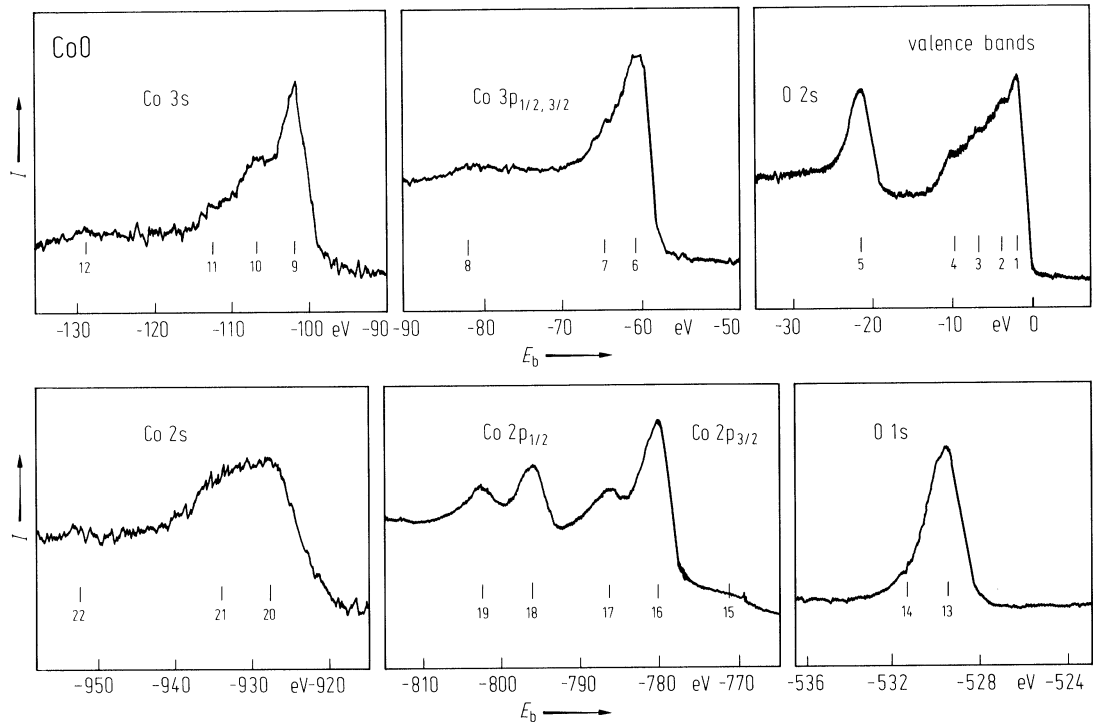

Fig. 4.

CoO. (a) Real and imaginary parts of the dielectric function vs. photon energy, (b) absorption coefficient vs. photon energy at RT [70P].

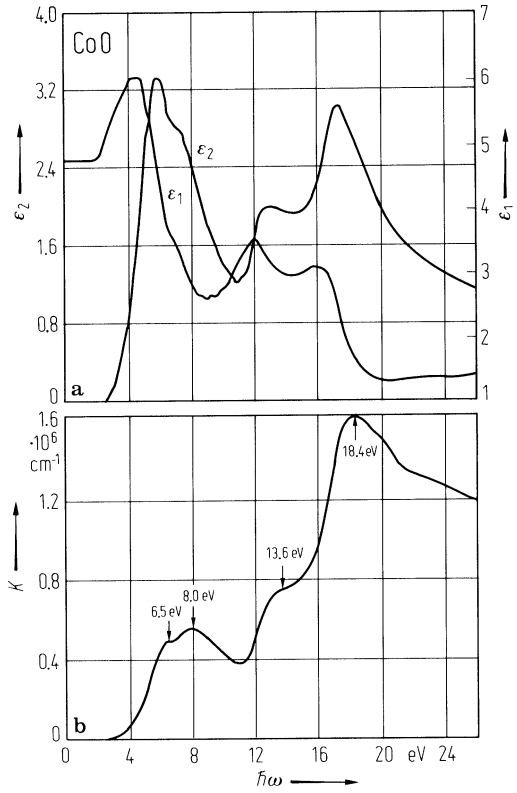

Fig. 5.

CoO. Thermoreflectance vs. photon energy at various temperatures [72M2].

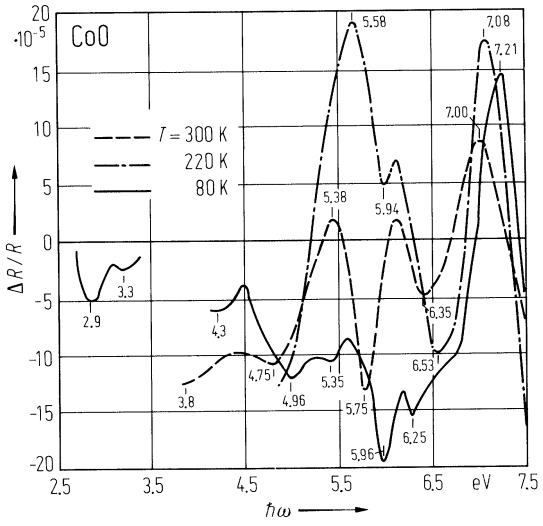

Fig. 6.

CoO. Empirical energy level diagram (RT data). Left: band states, right: localized states derived mostly from data at 80 K [72M2]. For assignment of states, see table.