

Electron structure and correlation effects in high- T_c superconductors and transition metal oxides

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1. Introduction

In spite of some successes of one-electron spin-polarized band structure calculations to describe the electron structure of high- T_c superconductors and 3d metal magnetic monoxides as a whole, they do not reproduce band gap values and underestimate values of local magnetic moments. The comparison of such calculations with XPS and UPS data shows that a discrepancy of about 1–2 eV is observed in respect of position of valence band about Fermi level.

It is asserted that one-particle band structure theory is not applicable to the analysis of electron structure and magnetic properties of the compounds with strong electron-electron correlation. In this connection the attempt of a rehabilitation of one-electron band structure methods for such purposes is of great interest.

2. Method of calculation

The method of accounting for the correlation effects in band structure calculations by introducing the self-interaction correction (SIC) was proposed by Perdew and Zunger (1981). In SIC method, the potential created by the charge density of the electron itself is subtracted from total LSDF potential that leads to lowering the energies of occupied states and, in some cases, to opening of a band gap. The application of SIC to NiO gave the band gap about 4 eV which agrees with experimental value (Sawatzky and Allen 1984) but was accompanied by a redistribution of states in the valence band contradicting the photoemission data.

It means that the use of the SIC method allows one to decrease by one the number of electrons interacting with an electron in the valence band, thus providing different potentials for electrons in the valence and conduction bands. However, the energies of different occupied states get lower in a non-uniform way which can lead to redistribution of the valence band states and hence to distortion of the ground state results.

In our method it is also possible to obtain the required difference of potentials for electrons of valence and conduction bands. But in contrast to the SIC method, in the present case, the number of electrons acting on the electrons in occupied states remains unchanged, and the number of electrons with which an electron in conduction band interacts is increased by one. It leads to the opening of band gap as in the SIC method, but it is not accompanied by any distortion of the ground-state characteristics

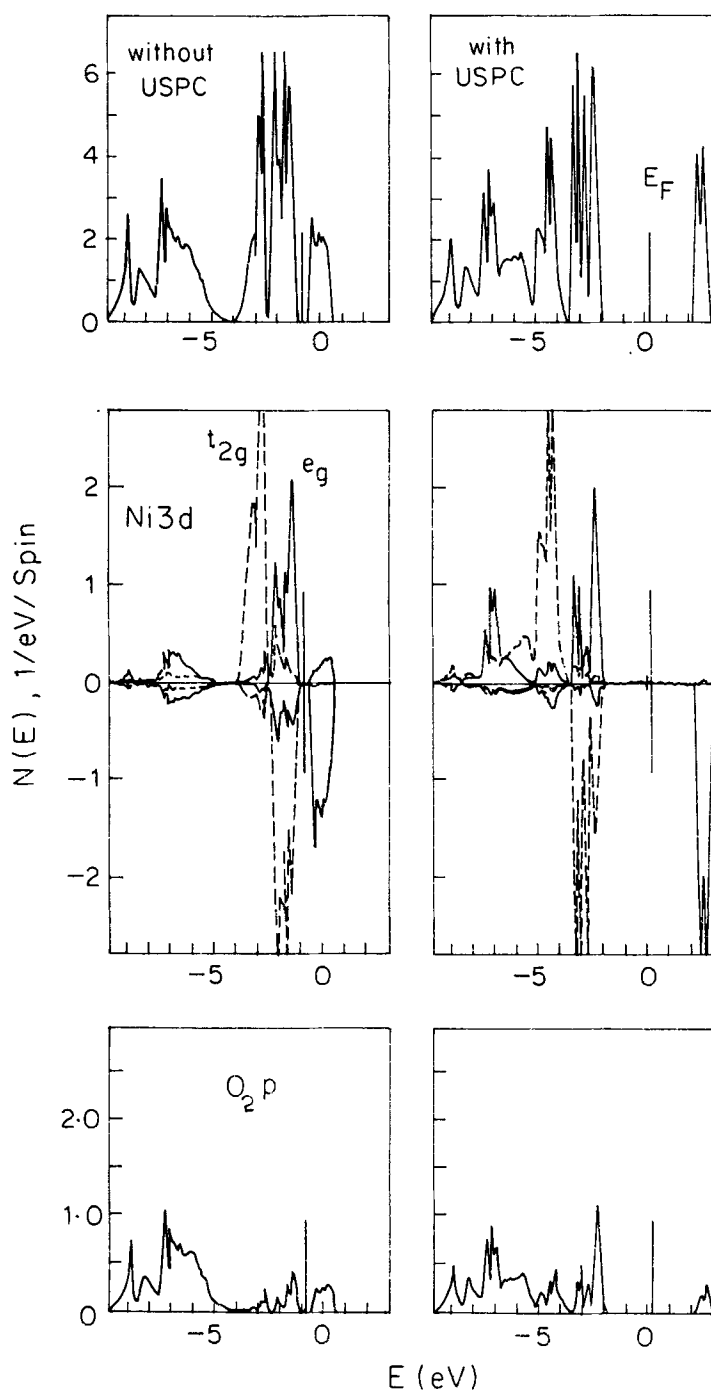


Figure 1. Total (upper row) and partial densities of states for NiO, with and without USPC band structure calculations.

because the potential for valence band states does not change. We named this method "unoccupied states potential correction" (USPC). The details of implementation of the USPC method within the LMTO-ASA calculation scheme, were given earlier (Anisimov *et al* 1989, 1990).

3. Results

The results of experimental values of band gaps and local magnetic moments obtained for magnetic oxides and La_2CuO_y , CaCuO_2 , $\text{Sr}_2\text{CuO}_2\text{Cl}$ are presented in tables 1 and 2. Also listed for comparison are data obtained by Terakura *et al* (1984). An

Table 1.

Compound	Energy gap (eV)		
	Theory		Experiment
	Without USPC	With USPC	
MnO	0.82	3.59	3.6–3.8
FeO	0	2.50	—
CoO	0	2.66	3.0
NiO	0.41	3.90	4.0–4.3
La_2CuO_4	0	0.78	—
CaCuO_2	0	1.1	—
$\text{Sr}_2\text{CuO}_2\text{Cl}_2$	0	2.0	—

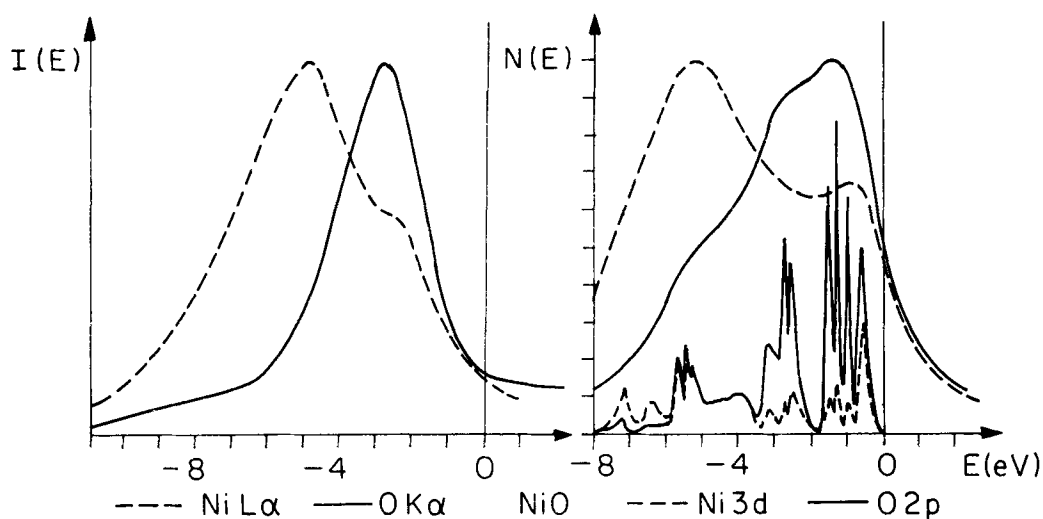


Figure 2. Comparison of partial $\text{Cu } 3d$ and $\text{O } 2p$ densities of states distribution (smearred for experimental distortion and width of inner level) and XES of compound for NiO.

analysis of these results leads to the conclusion that the suggested USPC-method gives an opportunity to obtain for the first time reasonable agreement with experiment within the frame of the LSDF-approach.

The results of spin-polarized band structure calculations using USPC correction for NiO are presented in figure 1. We also performed X-ray emission spectra (XES)

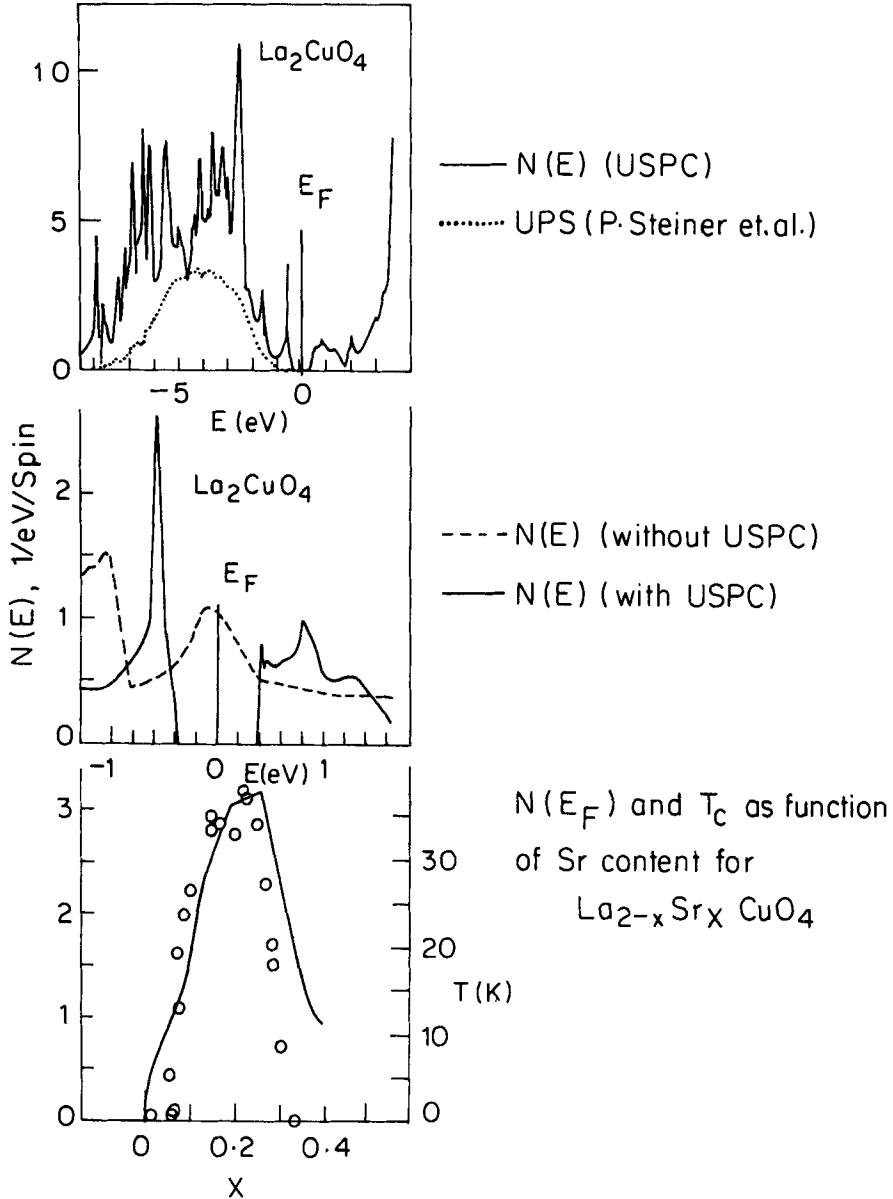


Figure 3. (a) Total density of states for antiferromagnetic La_2CuO_4 . (b) Sum of the copper and plane oxygen densities of states for La_2CuO_4 in the energy region near the Fermi level. The full line corresponds to antiferromagnetic solution, and the dashed line to nonmagnetic solution. (c) Calculated dependence of the density of states at the Fermi energy on x for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (solid line) and experimental data for T_c (squares) (Cheong *et al* 1989).

Table 2.

Compound	Local magnetic moments (B)			
	Theory			Experiment
	Without USPC		With USPC	
	Terakura <i>et al</i> (1984)	Our results		
MnO	4.45	4.47	4.74	4.79
FeO	3.43	3.42	3.42	—
CoO	2.35	2.29	2.70	3.35
NiO	1.09	1.05	1.68	1.64–1.77
La ₂ CuO ₄	—	0	0.38	0.40
CaCuO ₂	—	0	0.54	0.51
Sr ₂ CuO ₂ Cl ₂	—	0	0.67	0.34

measurements for FeO, MnO and NiO. The experimental conditions of these measurements were given by Galakhov *et al* (1989). The results obtained for NiO are compared with band structure calculations (see figure 2). The local density of O_{2p} and Me_{3d} states distribution is smeared by total experimental distortion (instrumental distortion + width of inner level). The relative position of O_{2p} and Me_{3d} bands is reproduced by XES (XES of compounds are combined in one energy scale with the help of XPS-measurements of O_{1s} and Me_{2p} binding energies).

The total density of states for antiferromagnetic La₂CuO₄ is shown in figure 3. The use of USPC results in band gap and also in the semiconducting character of the ground state. Doping of Sr in the "rigid band" model corresponds to the lowering of Fermi energy and leads to a sharp increase in the N(E_f) and N(E_f) reaches a maximum at $x = 0.20-0.25$. The dependence of N(E_f) on Sr concentration x thus obtained correlates with experimental values of T_c (Cheong *et al* 1989) for La_{2-x}Sr_xCuO₄. In both cases the maximum is reached at the value of $x = 0.2 - 0.25$ there is a sharp increase in the region of $x = 0.05 - 0.15$ and a sharp decrease for $x = 0.25 - 0.35$. Such a correlation is typical for superconductors, for instance, for A-15 type compounds.

References

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