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Optical properties of non-centrosymmetric Th-based superconductors: a density functional theory study

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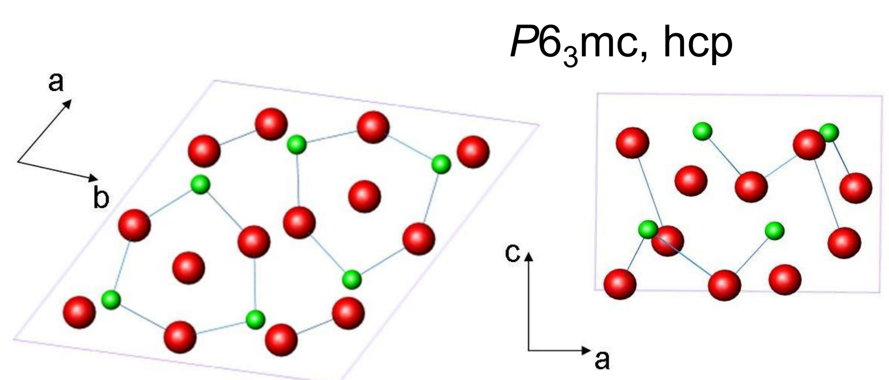
INTRODUCTION & AIM

Non-centrosymmetric superconductors are intensively studied due to the fact that the lack of inversion center could lead to a mixed state of the spin-singlet and spin-triplet configurations of the superconducting pairs[1]. The investigation of optical properties with the help of electronic transitions will be presented for non-centrosymmetric superconductors based on Th with the stoichiometry Th_7T_3 (T=Fe, Co, Ni) [2-5], exhibiting weak electron correlations. The studied Th_7T_3 compounds, crystallizing in the hexagonal Th_7Fe_3-type structure (space group P63mc), undergo transition into a superconducting state at $T_c \approx 2$ K. The crystal unit cell is characterized by the three atomic positions for thorium atoms with Th1, Th2 located at 6c positions and Th3 at the 2b position and one position (6c) for the transition metal. By replacing the Fe with Co or Co by Ni one additional electron was added to the system. This substitution of one atom of transition metal to another related with change in the atomic masses and also the role of relativistic effect of thorium atoms lead some interesting properties to the electronic structure and optical properties of Th_7T_3 compounds. We emphasize on the role of the ASOC strength since anisotropic spin splitting, both in the band structure and optical properties emerge when one takes into account the spin-orbit coupling in the calculations.



Th_7T_3	Lattice parameteres (nm)	T_C (K)
Th_7Fe_3	$a = b = 0.9849$ $c = 0.6198$	1.98
Th_7Co_3	$a = b = 0.9863$ $c = 0.6252$	1 .81
Th_7Ni_3	$a = b = 0.9890$ $c = 0.6228$	1.94

Atomic positions:

Th1	**6c**	x, -x, z
Th2	**6c**	x, -x, z
Th3	**2b**	1/ 3, 2/3, z
T	**6c**	x, -x, z

METHOD

Electronic structure calculations for Th_7T_3 were performed using the full-potential linearized augmented plane wave (FP-LAPW) method [6]. The exchange–correlation effects were treated within the local density approximation (LDA) using the Perdew–Wang parameterization [7]. Self-consistent calculations of the electronic charge density were carried out employing the tetrahedron integration scheme with an (8 × 8 × 12) k-point mesh, corresponding to 768 k-points in the irreducible Brillouin zone.

Since the optical properties reflect the electronic structure of a system, it is of interest to interpret the main features of the optical spectra in terms of the electronic transitions in the studied materials. We will treat the optical properties as expressed by the frequency-dependent dielectric function associated with direct interband transitions.

ELK calculates the frequency dependent dielectric matrix after the electronic ground state has been determined. The imaginary part is determined by a summation over empty states using the equation:

$$\varepsilon^{(2)}_{\alpha\beta}(\omega) = \frac{4\pi^2 e^2}{\Omega} \lim_{q\to 0} \frac{1}{q^2} \sum_{c,v,\mathbf{k}} 2w_{\mathbf{k}} \delta(\varepsilon_{c\mathbf{k}} - \varepsilon_{v\mathbf{k}} - \omega) \times \langle u_{c\mathbf{k}+\mathbf{e}_\alpha q} | u_{v\mathbf{k}} \rangle \langle u_{c\mathbf{k}+\mathbf{e}_\beta q} | u_{v\mathbf{k}} \rangle^*,$$

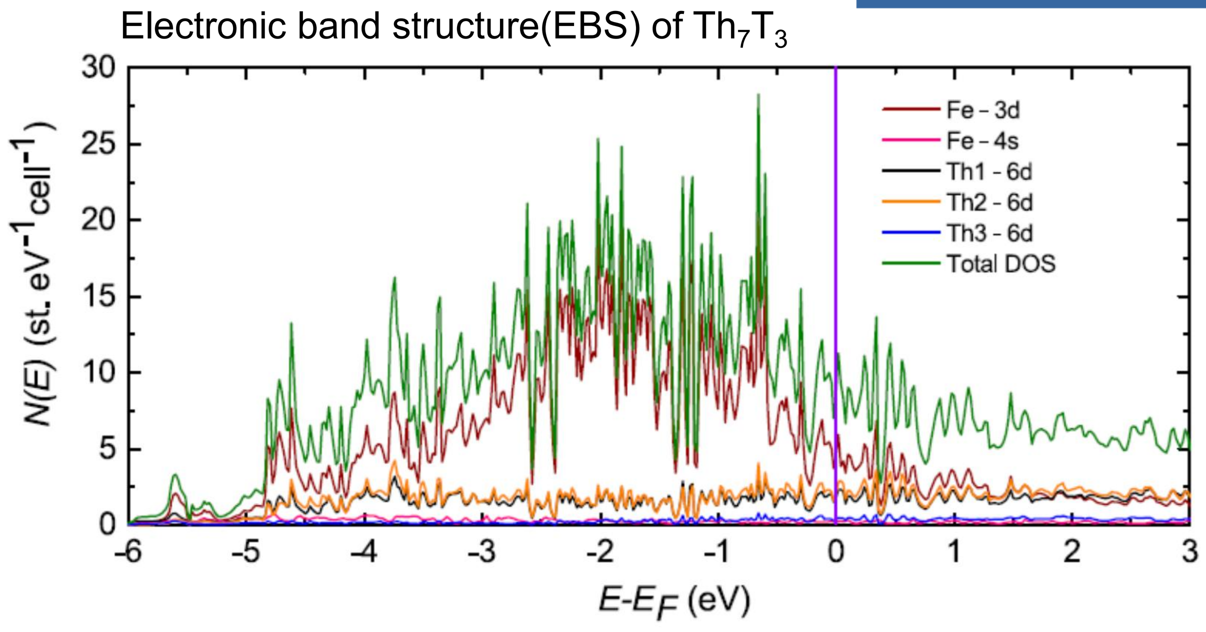
where the indices c and v refer to conduction and valence band states respectively, and u_{ck} is the cell periodic part of the orbitals at the k-point k.

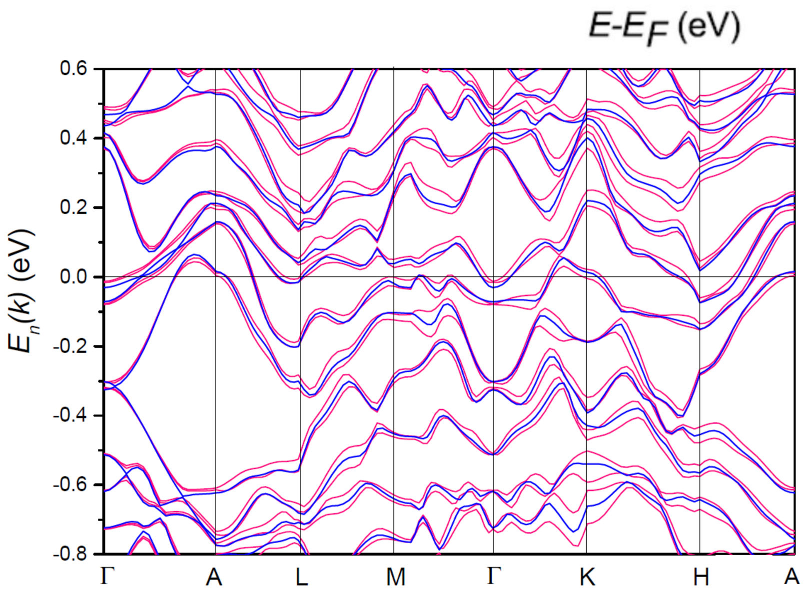
The real part of the dielectric tensor is obtained by the usual Kramers-Kronig transformation, where *P* denotes the principle value.

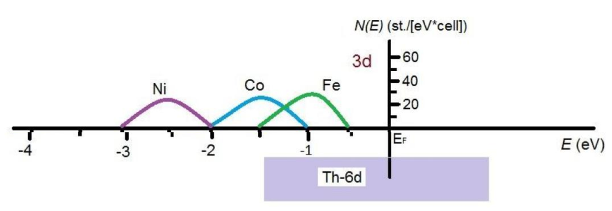
$$\varepsilon^{(1)}_{\alpha\beta}(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\varepsilon^{(2)}_{\alpha\beta}(\omega')\omega'}{\omega'^2 - \omega^2 + i\eta} d\omega'$$

RESULTS & DISCUSSION

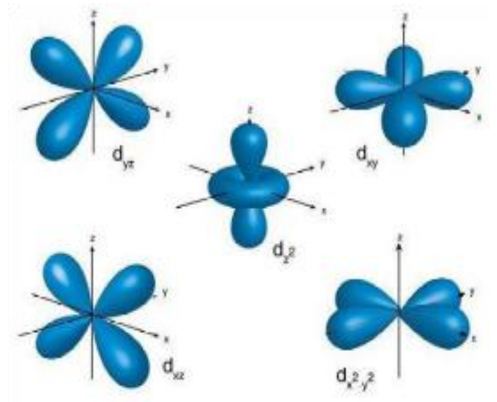
Electronic band structure(EBS) of Th_7T_3

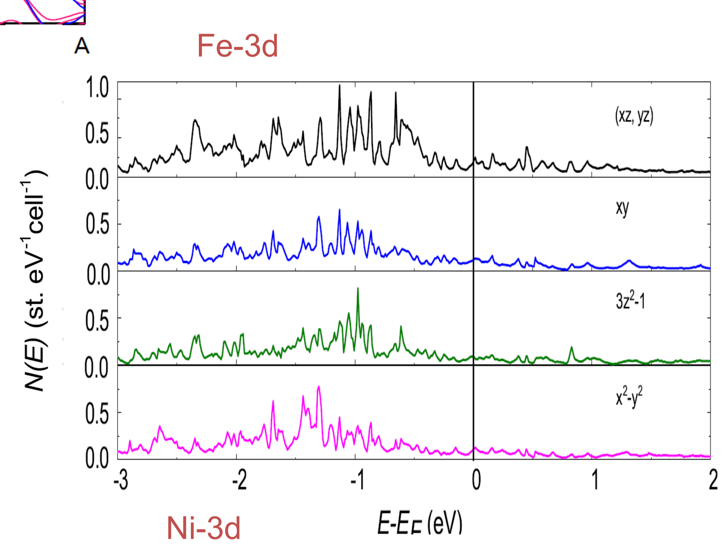


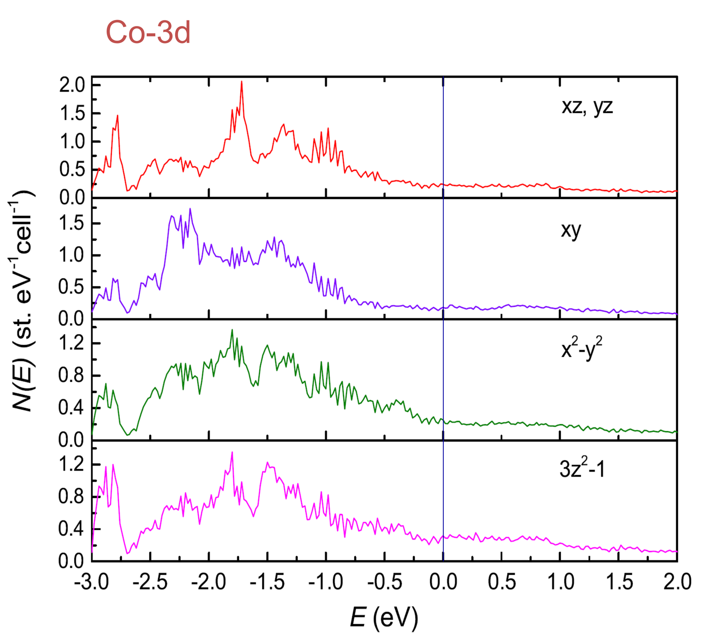


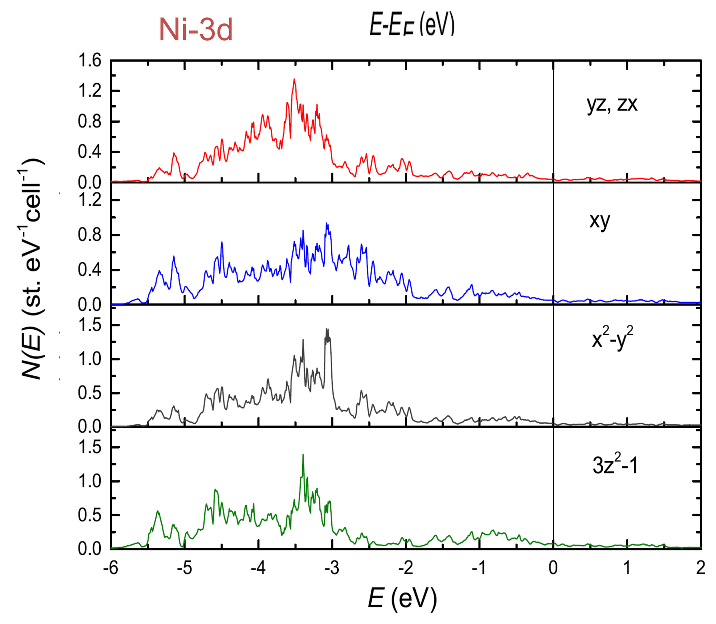


Th_7T_3	ΔE_{split} (meV)	
	FP-LMTO	FP-LAPW
Th_7Fe_3	40-100	30-100
Th_7Co_3	30-100	30-90
Th_7Ni_3	10-30	10-40

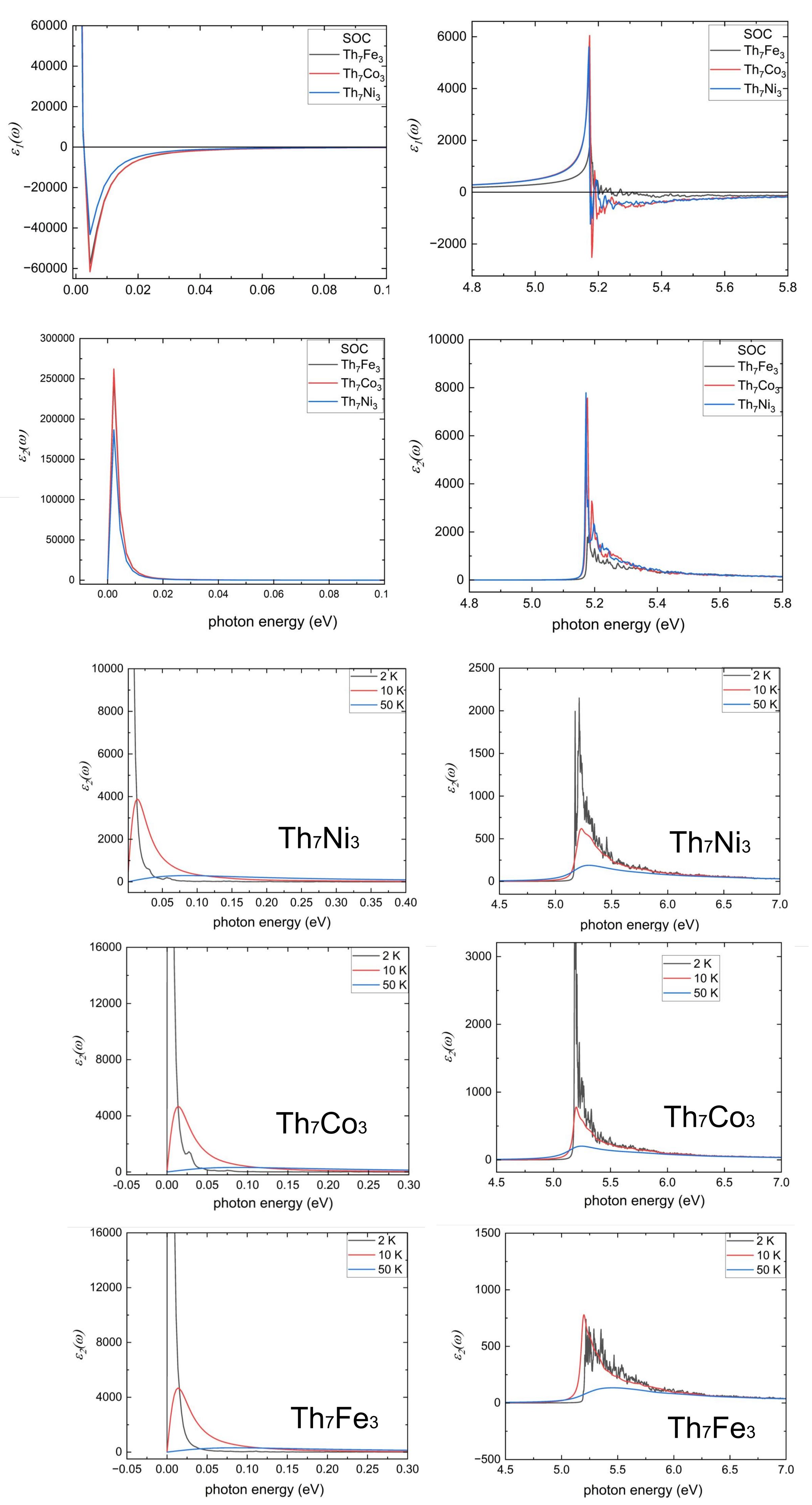


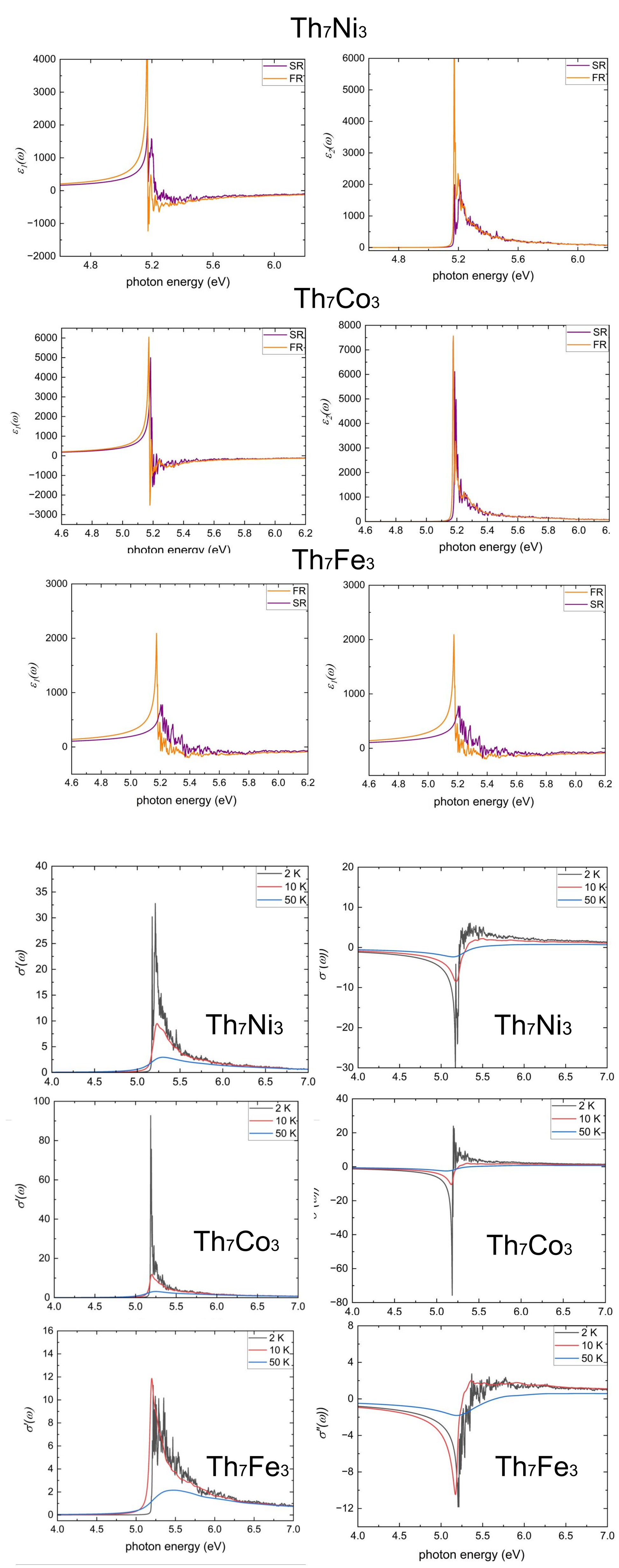






Dielectric function and optical conductivity of Th_7T_3





CONCLUSIONS

The optical response of the weakly correlated non-centrosymmetric superconductors Th_7T_3 (T = Fe, Co, Ni) was investigated within both scalar-relativistic (SR) and fully relativistic (FR) approaches. The compounds exhibit a pronounced low-energy intraband contribution and a strong interband transitions around 5–6 eV, indicating significant optical absorption in the ultraviolet region.Comparison between SR and FR calculations reveals that spin-orbit coupling modifies the interband transitions and leads to anisotropic spin splitting, highlighting the importance of relativistic effects in the optical properties of Th-based non-centrosymmetric superconductors.

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