IL NUOVO CIMENTO **48 C** (2025) 205
DOI 10.1393/ncc/i2025-25205-0

COMMUNICATIONS: SIF Congress 2024

Spin-filters magnetic transparent conductors(*)

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received 12 June 2025

Summary. — Transparent Conductors (TCs) exhibit optical transparency and electron conductivity, the most common being electron-doped oxides. By searching for non-oxides TCs, able to accept transition metals as doping elements without loosing their key characterstics, we extend this class of systems to the magnetic realm and introduce new functional materials that combine transparency and conductivity with magnetic spin polarization opening the way to spintronic applications, such as spin filters.

1. – Introduction

Transparent conductors (TCs) show high transparecy and large electrical conductivity at the same time. This unusual combination makes them unique and particularly suitable for a large variety of appications in the field of optoelectronics. The most common TCs are heavily doped wide-bandgap metal oxides (TCOs), such as indium tin oxide (Sn:In_2O_3, ITO), aluminum zinc oxide (Al:ZnO, AZO), and fluorine tin oxide (F:SnO_2, FTO) [2]. The extension of transparent conductivities to magnetic materials would open up the integration into transparent spintronic applications [3] and spin manipulation through electronic and/or optical interactions, such as field effect, spin filtering and photo carrier injection [4]. Doping metal-oxides with magnetic transition metal (TM) elements would seem the easiest way to impart a magnetic character to TCs. However, the high chemical affinity between the *d*-orbitals of TMs and oxygen states often results in localized chemical bonds and the emergence of mid-gap states (*i.e.*, no free-charge donation), which are detrimental for both the conductivity (carrier traps) and the transparency (optical interband transitions) of the system. To overcome the limitations in TCOs, we exploit high-throughput *ab initio* methodologies, in order to identify a set of non-oxides TCs that show additionally spin-filtering properties once doped with TMs.

(*) This article is a short overview of D'AMICO P. *et al.*, *Acta Mater.*, **289** (2025) 120850, https://doi.org/10.1016/j.actamat.2025.120850, see ref. [1].

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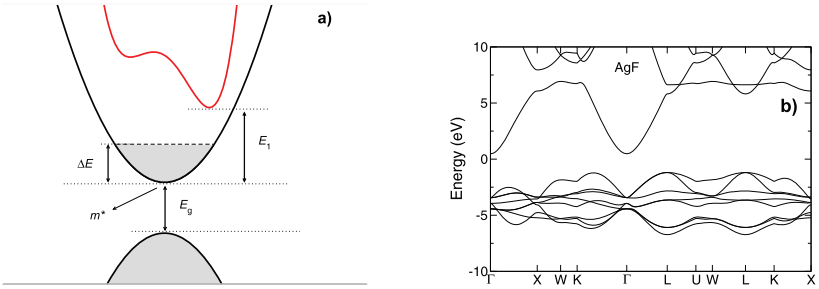

Fig. 1. – (a) Sketch of a prototypical TC band structure highlighting the essential parameters used as descriptors as described in eq. (1). Gray areas identify the occupied bands of the doped system. (b) Band structure of one of the filtered and investigated host materials, AgF.

2. – Methods

First principles calculations have been performed within local-spin-density approximation and the DFT+U framework, by using the Quantum Espresso suite [5] and the ACBN0 approach [6]. The optical properties have been calculated with the *epsilon.x* code, also included in the Quantum Espresso suite, evaluating the complex dielectric function $\hat{\epsilon}(\omega)$ within the standard Drude-Lorentz approximation [7]. The electrical spin conductivity σ^s ($s = \{\uparrow, \downarrow\}$) is evaluated by using the PAOFLOW code [8] that solves the Boltzmann equation for transport in the relaxation-time approximation.

3. – Results and discussion

We start by characterizing the TCs with physical descriptors, that we define by taking ITO and AZO as guiding prototypes and then use them to search for promising TCs included in the AFLOW repository [9, 10]. In fig. 1(a) we sketch the electronic band structure of a prototypical TC and its physical descriptors: the band gap E_g, that has to be large enough to achieve transparency; the effective mass m^*, directly related to the conductivity of the electrons injected in the conduction through n-doping; the energy difference E_1 between the first and second conduction bands, that needs to be large enough in order to preserve the transparency after doping. By taking into account the well-known underestimation of the bandgap in DFT and considering ITO and AZO as reference TCs we impose the following filters to the AFLOW database:

$$\begin{aligned} E_g &> \quad 1.0 \text{ eV}, \\ m^* &< \quad \frac{1}{2} m_0, \\ E_1 &> \quad 2.0 \text{ eV}. \end{aligned} \tag{1}$$

No conditions are instead imposed on the chemical composition of the materials. The descriptors expressed in eqs. (1) were used to scan the full AFLOW database resulting in a list of 115 potential TCs [1] and in fig. 1(b) we report the band structure of a filtered system, AgF, to show the close similarity to the model one.

We focus our attention on binary compounds and we restrict our search on TM-halides (AgF, AgCl, CuCl, $CdCl_2$) and on an alkali chalcogenide (Na_2S), that are representatives

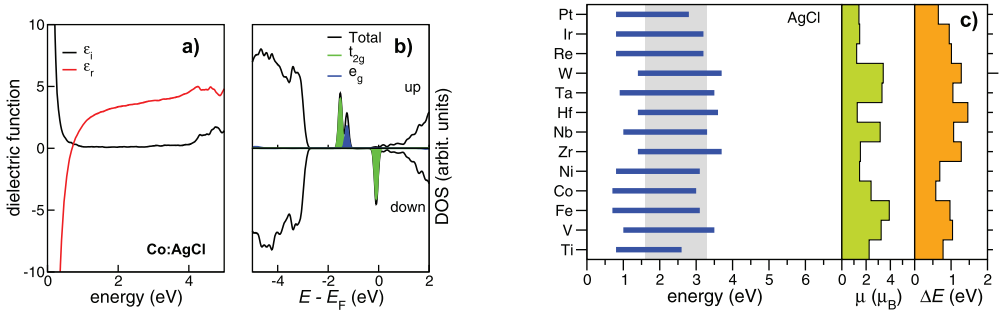

Fig. 2. – In (a) and (b) the complex dielectric function and the DOS of Co:AgCl are reported, respectively. (c) Energy distribution of the optical transmittance $T(E)$ (left panel), total magnetization μ (central panel), and ΔE (right panel) for TM:AgCl. Blue horizontal lines identify the transparency range $T(E) > 0.9$; the shaded gray area indicates the visible range. Only the TM-host systems that satisfy the three conditions $\{\mathcal{C}_i\}$ are reported.

of different gap type, anion/cation valence, and stoichiometry. We then add —one-by-one— all 30 TMs elements to the system as metal-substitutional defects. For each system we evaluate the position of the Fermi level ΔE, the total magnetization and the transmittance T(E) (expressed in terms of the dielectric function) imposing the following conditions in order to be considered as magnetic TCs (MTCs):

$\mathcal{C}_1$) the Fermi level lies above the top of the first conduction band, so $\Delta E > 0$;

$\mathcal{C}_2$) the transmittance is close to unity ($T(E) > 0.9$) in the visible range that corresponds to have a transparent system;

$\mathcal{C}_3$) the total magnetization μ is greater than zero.

The results of the HT search are summarized in fig. 2 for AgCl. On panels (a) and (b) we show the dielectric function and the density of states (DOS) for the case of Co:AgCl: the dielectric function has the typical Drude-like shape and there is an imbalance in the occupation of the spin-up and spin-down states, resulting in a finite magnetization ($\mu = 2.24\ \mu_0$/cell). The spin-up spectrum has two sharp peaks within the host bandgap. These correspond to the t_{2g} and e_g orbitals that Co forms within the cubic crystal field in the host (green and blu areas, panel (b)). On fig. 2(c) we report in a compact form, for each dopant, the frequency regions where $T(E) > 0.9$ (blue bars) and the visible range (gray area), the total magnetization and the ΔE demonstrating that TC properties can cohexists with a finite magnetization. A key role for the electron transport is played by the energy alignment among E_F, the spin-polarized orbitals, and the conduction band where the relative energy positions gives rise to two possible scenarios. If the orbitals are degenerate with E_F there is a spin-imbalance resulting in different spin-conductivites (spin filter) otherwise the conducting properties are spin-independent (no spin filter). This difference can be illustrated comparing V:AgCl and Fe:AgCl: the energy alignments of the spin-polarized states in the DOS (fig. 3(c)) result in different spin-polarized conductivities as shown in fig. 3(a). We quantify this difference by defining the spin conduction polarization

$$P = \frac{\sigma^{\uparrow} - \sigma^{\downarrow}}{\sigma^{\uparrow} + \sigma^{\downarrow}}, \tag{2}$$

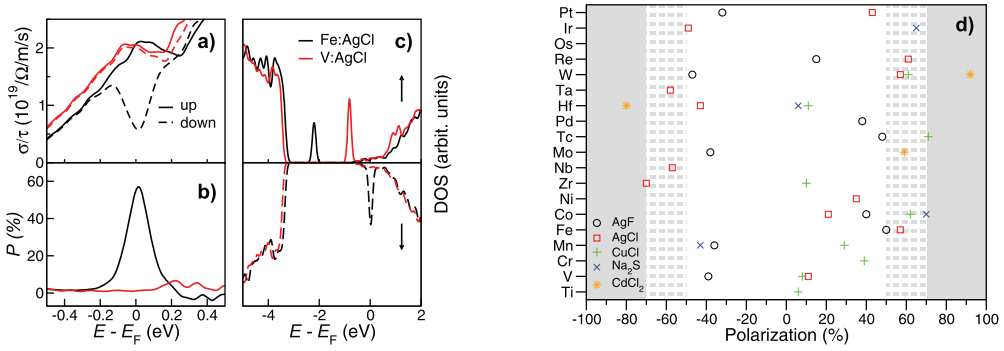

Fig. 3. – (a) Conductivity, (b) spin-polarization, P, and (c) DOS for Fe:AgCl (black curves) and V:AgCl (red curves). Spin-up and spin-down components are represented by solid and dashed lines respectively. (d) Maximum value of the spin-polarization for all the dopant-host systems, where the hosts are the five selected ones in the full list. The light-grey and the dark-grey areas indicates the ranges $50\% < \|P\| < 70\%$ and $70\% < \|P\| < 100\%$, respectively.

and in fig. 3(b) we can see that Fe:AgCl acts as a good spin filter, blocking more than $\simeq$ 60% of spin down electrons while V:AgCl is not. By computing the polarization P for each MTCs we identify the combinations that are also suitable for spin-filter applications. The results are summarized on fig. 3(d), where for each MTC, we report the maximum value of $P \neq 0$. In light(dark)-grey we highlight the ranges where $\|P\| > 50\%(70\%)$, that can be considered to represent a good (very good) spin-filter.

4. – Conclusions and perspectives

We theoretically predicted a novel class of non-oxide materials, namely magnetic transparent conductors, that merge the optical and transport properties typical of TCs and a net magnetic moment. By doping with transition metal element and characterizing the electronic and optical properties of the resulting MTC systems we identified a set of MTCs that exhibit a large spin conduction polarization up to $\simeq$ 90%. Future research, exploring the effect of the doping percentage, could lead to the inclusion of new systems in the identified set. The present discovery may open new routes for application of TC compounds as spin filters in spintronic devices.

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The author acknowledges all the co-authors of the original work [1].

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