Effect of Chromium in Ytterbium Monoxide towards Spintronics Application

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Introduction

- ✓Investigations haave indicated that the electron spin can be controlled, and therefore explored for many spin-based devices (especially data storage).
- ✓Spin based data storage devices have multifunctional characteristics such as:
  - non-volatility
  - high data-processing speed
  - higher integration densities
  - extremely low dynamic power consumption
- ✓Magnetic semiconductors are particularly attractive due to their capacity as non-volatile memories and magneto-optical devices such as optical switches and other devices where spin injection sources of electrons are important.
- ✓Many magnetic semiconductors can be realized when III-V, II-VI or IV-VI semiconductors are doped with magnetic elements such as Fe and Ni.

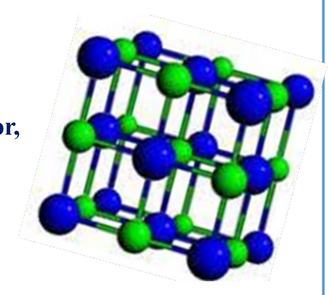
Technological applications of alkaline and alkaline earth chalcogenides are wide and have been well elucidated. Lanthanide chalcogenides are not well known because the lanthanides ions have a stable 3+ valence.

Among the lanthanides, Europium (Eu) and Ytterbium (Yb) have larger ionization energies and can thus form stable lanthanide chalcogenide. While Europium oxide (EuO) and Europium sulfide (EuS) are commercially available and used as fluorescent material, less reports are available for ytterbium compounds.

Photo-voltaic Thermoelectric

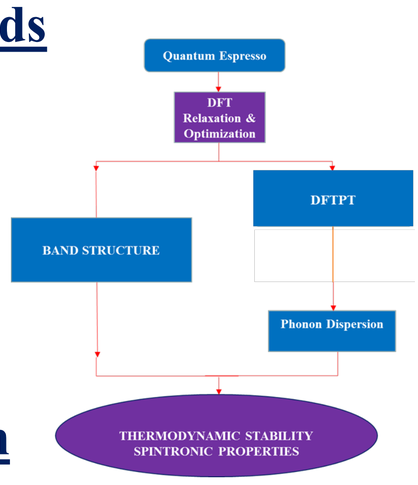
However,

- ➢Ytterbium (II) Oxide (YbO) have been predicted/synthesized a semiconductor, crystallizing in a stable nonmagnetic rock-salt NaCl-type (B1) structure at ambient conditions.
- ➢Viable technological applications yet to be identified for YbO.



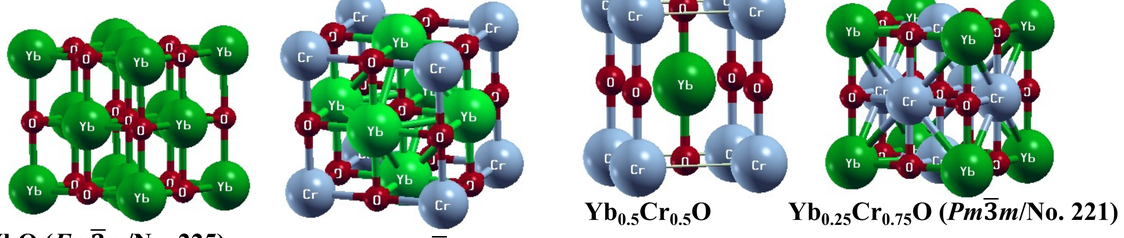
Calculation Methods

- ➢The Density Functional Theory (DFT) implemented in the Quantum Espresso package was used.
- ➢The exchange and correlation potential was evaluated by the generalized gradient approximation of Perdew-Burke- Enzerhof
- ➢The structure, electronic performance, magnetism and stability of $Yb_{1-x}Cr_xO$ were investigated at concentrations of x = 0, 0.25, 0.5 and 0.75.
- ➢To check for dynamic stability, the density functional perturbation theory was used to calculate the phonon frequencies for each concentration.



Results & Discussion

Crystal structures



YbO ($Fm\bar{3}m$/No. 225) $Yb_{0.75}Cr_{0.25}O$ ($Pm\bar{3}m$/No. 221) $Yb_{0.5}Cr_{0.5}O$ ($P4/mmm$ - No. 123) $Yb_{0.25}Cr_{0.75}O$ ($Pm\bar{3}m$/No. 221)

Equilibrium Properties and Thermodynamic Feasibility

$$E_{FM} = E_{total}(Yb_{4-x}Cr_xO_4) - \left(\frac{(4-x)\,E(Yb)}{8}\right) - \left(\frac{x\,E(Cr)}{8}\right) - \left(\frac{4\,E(O)}{8}\right) \quad \textbf{(1.0)}$$

Table 1: The result of the formation energy (E_{FM}) as calculated using equation (1.0)

Conc.	E_{FM} (Ry)
$Yb_{0.75}Cr_{0.25}O$	-502.429
$Yb_{0.5}Cr_{0.5}O$	-179.752
$Yb_{0.25}Cr_{0.75}O$	-565.792

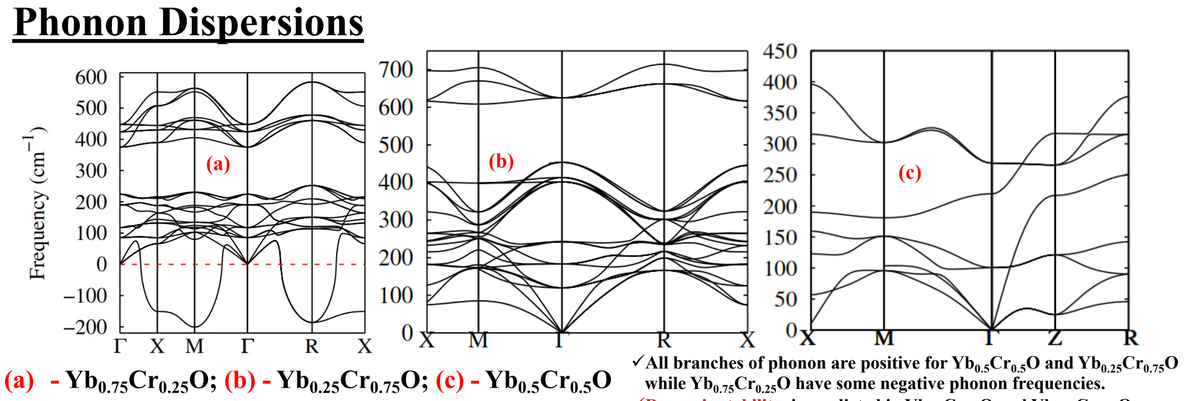
Table 2: The result of calculated equilibrium lattice parameters (LP), bulk modulus (B) and its pressure derivative (B') for $Yb_{1-x}Cr_xO$.

Conc.	LP (Å)	B (GPa)	B'
YbO	4.722, [4.88][a], 4.743[b]	121.6, [130 ± 10][a], 128[b]	4.45 [4.0][a]
$Yb_{0.75}Cr_{0.25}O$	4.567	256.6	6.61
$Yb_{0.5}Cr_{0.5}O$	a = 3.496, c = 0.643	421.0	15.50
$Yb_{0.25}Cr_{0.75}O$	4.325	533.2	14.42

[a]Expt. data from Refs. [3]; [b]PAW-GGA data from Ref. [4]

- ✓ The negative values of the formation energies (E_{FM}) calculated using equation (1.0) suggest that the compounds are thermodynamically stable in their respective structures.
- ✓ A good agreement exists between theoretical and experimental lattice constant, bulk modulus and the pressure derivative of bulk modulus for YbO.
- ✓ Based on the observation above, the data for the mixed compounds ($Yb_{1-x}Cr_xO$) should be reliable enough.
- ✓ The bulk modulus increases with increase in Cr content i.e. $Yb_{0.25}Cr_{0.75}O > Yb_{0.5}Cr_{0.5}O > Yb_{0.75}Cr_{0.25}O$

Phonon Dispersions

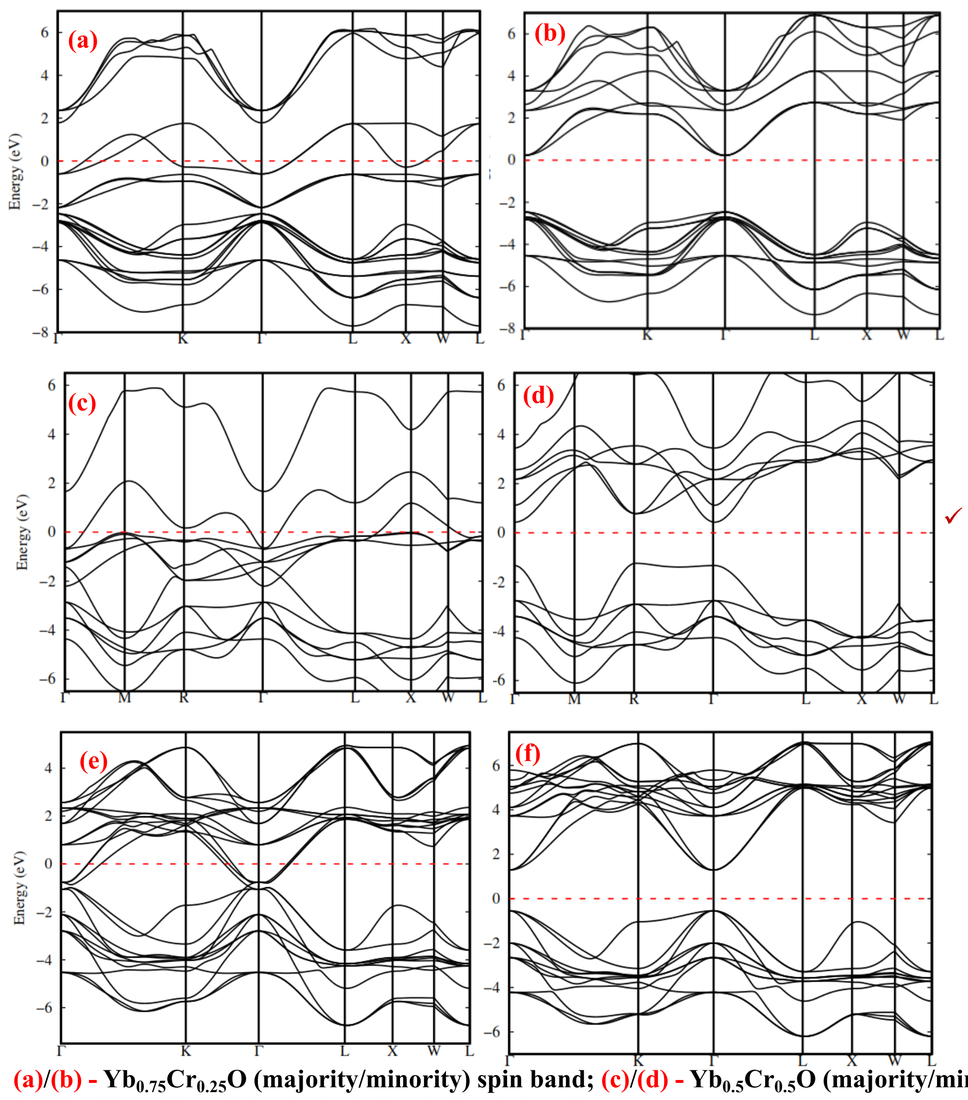


(a) - $Yb_{0.75}Cr_{0.25}O$; (b) - $Yb_{0.25}Cr_{0.75}O$; (c) - $Yb_{0.5}Cr_{0.5}O$

✓All branches of phonon are positive for $Yb_{0.5}Cr_{0.5}O$ and $Yb_{0.25}Cr_{0.75}O$ while $Yb_{0.75}Cr_{0.25}O$ have some negative phonon frequencies.

✓Dynamic stability is predicted in $Yb_{0.5}Cr_{0.5}O$ and $Yb_{0.25}Cr_{0.75}O$.

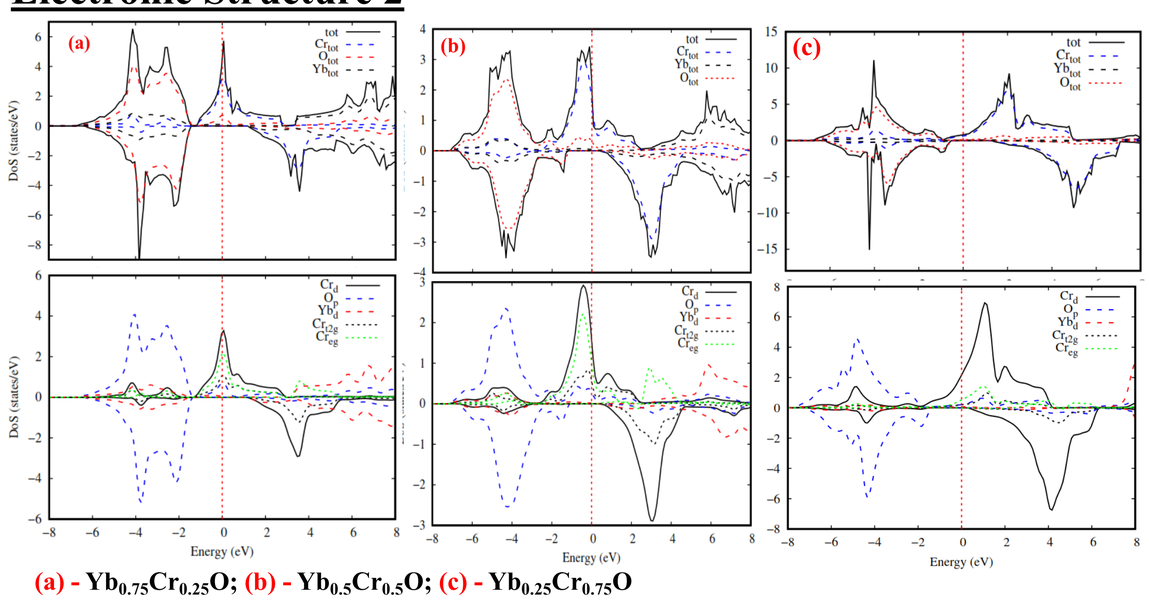
Electronic Structure 1



✓ All $Yb_{1-x}Cr_xO$ compounds show metallic and semiconductor (direct gap) characters respectively, for majority-and minority-spin bands.

(a)/(b) - $Yb_{0.75}Cr_{0.25}O$ (majority/minority) spin band; (c)/(d) - $Yb_{0.5}Cr_{0.5}O$ (majority/minority) spin band; (e)/(f) - $Yb_{0.25}Cr_{0.75}O$ (majority/minority) spin band

Electronic Structure 2



(a) - $Yb_{0.75}Cr_{0.25}O$; (b) - $Yb_{0.5}Cr_{0.5}O$; (c) - $Yb_{0.25}Cr_{0.75}O$

- ✓ All the compounds are metallic for majority spin and semiconductors for minority spin (100% spin polarization obtained).
- ✓ An asymmetric character is seen in the spin-polarized electronic structures, indicating that the compounds are magnetic.
- ✓ Magnetism is induced by the magnetic spins arising from the localized d-Cr majority-spin states.

Magnetic Properties

Table 3: Computed total and partial magnetic moments for Yb, Cr and O atoms and in the interstitial sites (in Bohr Magneton μ_B) for $Yb_{1-x}Cr_xO$ ($0.25 \leq x \geq 0.75$)

Conc.	Total	Yb	Cr	O	Interstitial
$Yb_{0.75}Cr_{0.25}O$	3.96	0.053	3.75	0.037	0.120
$Yb_{0.5}Cr_{0.5}O$	3.99	0.124	3.79	0.032	0.044
$Yb_{0.25}Cr_{0.75}O$	3.53	0.075	3.25	0.037	0.168

- ✓ The asymmetric character seen in the electronic structure 4 plots indicates that the compounds are magnetic in nature.
- ✓ The magnetism is induced by magnetic spins arising from the splitting of d-Cr to t2g and e2g in the majority-spin states.
- ✓ The positive partial magnetic moments for O atoms shows that its p-O states interact Ferro-magnetically with the d-Cr states.
- ✓ The positive partial magnetic moments of Cr and Yb atoms shows that their magnetic spins interact ferro-magnetically.

Conclusions

After the characterization of chromium induced ytterbium monoxide, $Yb_{1-x}Cr_xO$ ($0.25 \leq x \geq 0.75$), the following conclusions can be drawn:

- ✓ All compositions are dynamically and thermodynamically feasible.
- ✓ All $Yb_{1-x}Cr_xO$ ($0.25 \leq x \geq 0.75$) are direct gap ferromagnetic semimetal.
- ✓ The bulk modulus increased with increase in Cr concentration.
- ✓ The half-metallic ferromagnetic character are caused by the direct splitting of d-Cr orbitals.
- ✓ Being Magnetic Half-Metals (MHM) with 100% spin polarization, $Yb_{1-x}Cr_xO$ systems predicted suitable for exploration in spin-injection electronics (spintronics).

Acknowledgements

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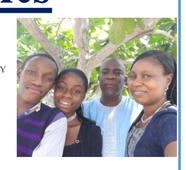

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