



People's Democratic Republic of Algeria
Ministry of Higher Education and Scientific Research
Kasdi Merbah Ouargla University
Department of Chemistry



1st international conference on chemical matters and environment preservation
IC-CMEP'22 March 09-10, 2022, Ouargla, Algeria (virtual conference)

N° :CP-403



Certificate of participation

The organizing committee of the 1st International Conference on Chemical matters and Environment Preservation
IC-CMEP'22 March 09-10, 2022, Ouargla – Algeria, certifies that:

Djamel ALLALI

Has successfully participated as a **POSTER** communication entitled:

Electronic and optical properties of Ag-based oxides XAgO (X= Li and Na): An ab initio study with the Tran–Blaha–modified Becke–Johnson density functional

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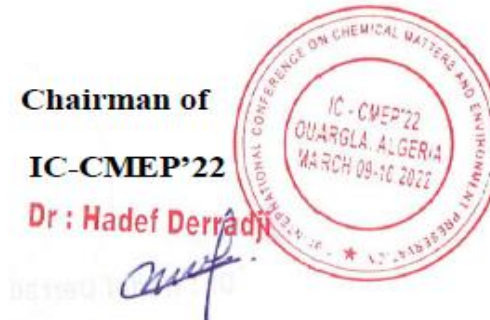
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Electronic and optical properties of Ag-based oxides XAgO (X= Li and Na): An ab initio study with the Tran–Blaha-modified Becke–Johnson density functional

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Abstract

We report ab initio density functional theory calculations of the structural, electronic and optical properties of Ag-based ternary oxides XAgO (X= Li and Na) using the full-potential linearized augmented plane-wave (FP-LAPW+lo) method [1] basis set as implemented in the WIEN2k code [2]. Calculated structural parameters, including the two lattice constants, (*a*) and (*c*), three internal coordinates, y_X , x_{Ag} , and x_O , bulk modulus (*B*) and its pressure derivative (*B'*), for the considered compounds using both the local density (LDA) [3] and generalized gradient approximations (GGA–PBESol) [4] are consistent with the available data in the scientific literature. To calculate the electronic properties, the exchange–correlation potential is treated with various functionals, and we find that the newly developed Tran–Blaha-modified Becke–Johnson (TB-mBJ) [5–7] functional significantly improves the band gap. Band structure, total and site-projected *l*-decomposed densities of states, charge-carrier effective masses, charge transfers and charge density distribution maps were obtained; analyzed and compared with the available theoretical data. The frequency-dependent complex dielectric function, absorption coefficient, refractive index, extinction coefficient, reflectivity and electron energy loss function spectra were calculated with an incident radiation polarized parallel to both [100] and [001] crystalline directions. The origins of the peaks and structures in the optical spectra are determined in terms of the calculated energy band structures.

Keywords: Ag-based oxides, *Ab initio* calculations, Structural parameters, Electronic properties, Optical spectra.

References

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Ministry of Higher Education and scientific Research

General Direction For scientific and technological development



1st International conference on Chemical matters and environment preservation

IC-CMEP'22 March 09 – 10, 2022, ALGERIA

Virtual Presentation



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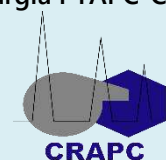
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Conference program

1st International conference on Chemical matters and environment preservation
IC-CMEP'22 March 9 – 10, 2022, ALGERIA

Conference Day 1 : Wednesday March 09, 2022		Time GMT+1
Opening ceremony	General Conference Chair Dr. HADEF Derradji, Univ. Ouargla (Algeria) https://meet.google.com/yyf-cqgu-hap	08 :30
	Pr. BECHKI Djamel, Dean of Mathematics & Matter Sciences Faculty (Algeria)	08 :45
	Pr. HALILAT Med Tahar, Ouargla University Rector (Algeria)	08 :55

Keynote speakers session

Session Chair Dr. BELFAR Med Lakhdar Ouargla University, Algeria		
Prof. BELKHALFA Hakim PTAPC-CRAPC- Ouargla	https://meet.google.com/yyf-cqgu-hap	09 :00
Prof DEKMOUCHE Messaouda Ouargla University, Algeria	https://meet.google.com/yyf-cqgu-hap	10 :00
Session Chair Dr. SAIDAT Mostapha Ouargla University, Algeria		
Prof. LEGHSEIR Belgacem Université Badji Mokhtar Annaba	https://meet.google.com/yyf-cqgu-hap	11 :00
Prof. MOUSSAOUI Younes Universté Gasfa tunisie	https://meet.google.com/yyf-cqgu-hap	11 :30
Session Chair Dr. Mazouz Mihoub Ouargla University, Algeria		
Prof. LANEZ Touhami Eloued University, Algeria	https://meet.google.com/yyf-cqgu-hap	12 :00
Prof ZENKHRI Louiza Ouargla University, Algeria	https://meet.google.com/yyf-cqgu-hap	12 :30

	Session Chair	Session Topic	Start discussion	Link (Google meet)
1	Pr. MOUSSAOUI Yassine	Eliminate environmental pollution (air, water and soil).	14:00	yacine.moussaoui@gmail.com
2	Dr. NDJIMI Mohammed Said	Nanomaterial's and the environment		nedjimi2011@gmail.com
3	Dr. Zerrouki hayat	Green chemistry and the environment Wastewater depollution.		zerroukih2020@gmail.com
4	Dr. Chaouch khaoula	Treat waste and preserve the environment		khaoula.chaouche@yahoo.fr
5	Dr. Rahmani zhor	Computational materials technique.		saouliibtissam@yahoo.fr
6	Dr. Ben Ali Moustapha	Crystalline structure modeling and optimization		meet.google.com/mdg-gded-sqg
7	Dr Saidat mustapha	Simulation and modeling of the physical and chemical properties of materials.		https://meet.google.com/yf-cqgu-hap
8	Dr. DAKMOUCHE Messaouda	Plants for the environment.		meet.google.com/eyb-hcdn-dpx
9	Dr. BOUZIANE Mebarka	Design of a new material synthesis technique.		bmebarka@yahoo.fr
10	Dr. Allaoui messaouda	Maters for optoelectronics.		https://meet.google.com/itf-vrvp-udp
11	Dr. BEN ZAHI Khadidja	Dielectric and magnetic maters		https://meet.google.com/oyo-ijfb-obb
12	Dr Allaoui abdelfetteh	Characterizations and applications of materials.		allaoui313@gmail.com
13	Dr Allaoui abdelfetteh	Materials for renewable energy.		allaoui313@gmail.com
14	Dr. SMARA Ouanissa	Organic and inorganic maters		ouanissasm@gmail.com
16	Dr. Mkhalfi tarek	Waste water depollution		https://meet.google.com/mzn-yfhh-vbs
17	Dr. Zaoui manel	Medical applications of new biomaterials and Nano-biotechnology.		https://meet.google.com/vwa-yycu-ocd
18	Dr. Hamada djamilia	Nanotechnology and Nanomaterials.		https://meet.google.com/dod-iwzu-qks

Conference Day 2 :Thursday March 10 , 2022

closing Session

Session Chair

Prof ZENKHRI Louiza, Ouargla University, Algeria

Google meet Link

Or

Presentation Youtube Link

09 :00

Closingremarks

09 :30