

ICPMSAM 2023

1st International Conference on Physico-chemistry,
Materials Sciences & Applied Mathematics
(ICPMSAM'23)

CERTIFICATE OF ATTENDANCE

(N°506912)

This Certificate that, **Ketfi Mohamed El Amine**
Has attended the conference on November 27-28, 2023 with the Oral presentation en-
titled: Theoretical analysis of structural, optoelectronic and magnetic properties
of ABO₂ Delafossite semiconductor
as the main author of this work.

Co-authors are respectively: Saber Saad essaoud

Chairman of the Conference



CONFERENCE CHAIR

Dr. BOUATROUS Mehieddin





Theoretical analysis of structural, optoelectronic and magnetic properties of ABO_2 Delafossite semiconductor

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KEYWORDS: *Delafossite, TB-mBJ, Magnetic properties, Dielectric function, Absorption coefficient and the reflectivity.*

ABSTRACT

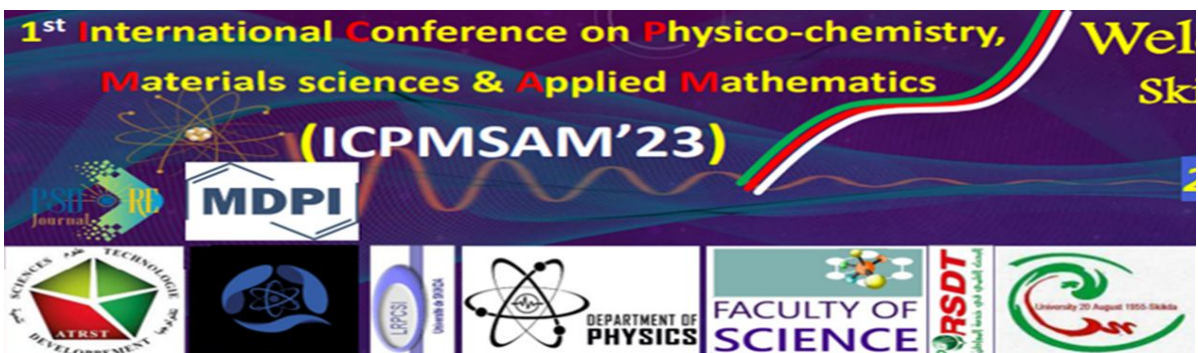
The Delafossite group of oxide materials was initially uncovered in 1965, comprising a category of ternary compounds characterized by the general formula ABO_2 , with A and B denoting metallic elements. One of the most prevalent Delafossites is $CuAlO_2$, which stands as a p-type semiconductor known for its remarkable electrical conductivity and transparency across the visible and near-infrared regions of the electromagnetic spectrum [1–3]. These distinctive qualities have propelled Delafossite materials into the spotlight for a wide array of applications, including use in electronic devices, energy storage, energy conversion, and optoelectronics. Their intriguing electronic, magnetic, and optical attributes have only recently garnered attention [4,5], prompting researchers to delve into these materials, not only to grasp their fundamental properties but also to uncover potential applications. Density functional theory (DFT) calculations have unveiled a range of electronic band structures within Delafossites, varying from metals to semiconductors contingent upon the specific choice of A and B ions. Furthermore, DFT calculations have forecasted that particular Delafossites, such as $CuCrO_2$ and $CuFeO_2$ [6,7], manifest antiferromagnetic ordering due to the interplay of spins on the transition metal ions. In an ab initio study conducted by Azmat et al. [8], it was demonstrated that $CuXO_2$ compounds (where X represents Al, Ga, In, B, La, Sc, Y) display semiconductive behavior. Experimental investigations into Delafossites have encompassed the electronic and optical properties. Among the most renowned Delafossites is $CuAlO_2$, renowned for its high electrical conductivity and optical transparency. $CuAlO_2$ boasts exceptional carrier mobility and low carrier concentration, making it an ideal candidate for transparent conductive electrodes in optoelectronic devices. Additionally, Delafossites have undergone scrutiny for their photovoltaic potential, with $CuInO_2$ and $CuGaO_2$ exhibiting promising results for solar cell applications. An experimental study by Kushwaha et al. [9] explored the $PdRhO_2$ compound, revealing its crystallization in a rhombohedral-type structure characterized by crystal cell dimensions of $a = 3.0240 \text{ \AA}$ and $c = 18.096 \text{ \AA}$.

In this study, we perform first-principles calculations based on density functional theory and the semi-classical Boltzmann method to investigate the structural, optoelectronic, magnetic, thermodynamic and thermoelectric properties for $BrCdO_2$ in the Tetragonal phase. To compute the structural properties, the Wang and the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA) was used as exchange-correlation potentials. Besides, the modified Becke-Johnson functional of Tran and Blaha (TB-mBJ) are used to compute the electronic and optical properties to achieve the best band gap energy values and a higher degree of precision. Our calculations have revealed that this compound have direct band gap 4.17 eV. As a result of this study, $BrCdO_2$ is promising material for optoelectronic devices, especially as photovoltaic materials in solar cells.



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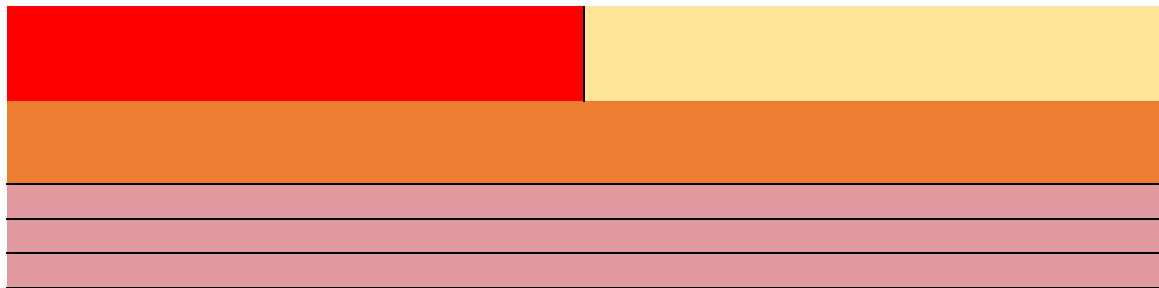
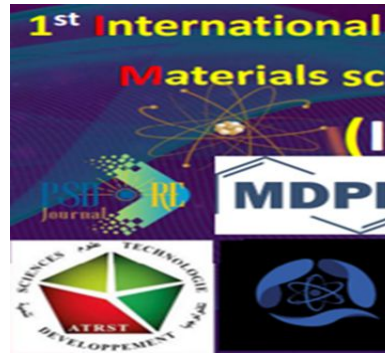
09:00-17:00	Registration				
09:00-09:05	Opening				
09:05-10:00	Protocol				
	Plenary session (chairman Loudi)				
10:15-10:45					
10:45-11:15	Pr.MERAD Ahcen				
11:15-11:44	Pr.Pierre francois brevet (online) lyon France				
11:45-12:25	Pr.CONSTANTINESCU Catalin-Danie (online) Marseille France				
12:00-13:00	Coffee break		Coffee break Coffee break		
		Chairman			Chairman
Time	Code	Room1	Time	Code	Room2
13:00-13:20		MOSBAH Salima	13:00-13:20		HADEF Zakaria
13:20-13:40		BOUSBA Housseem Eddine	13:20-13:40		BOUDIAR Abid
13:40-14:00		MOHAMMED BELHADJ Ahlem H	13:40-14:00		KHENNICHE Ghania
14:00-14:20		DJEGHLOUL Fatima	14:00-14:20		BENAISSA Amina
14:20-14:40		LASMI Sofiane	14:20-14:40		BENTRIDID Salah eddine
15:30-16:00					
16:00-16:30					
16:30-17:00					
		Chairman			Chairman
Time		Online1	Time	Code	Online2
17:00-17:20		ABDEL DJEBAR Hasnia	17:00-17:20		DAHO Salah Eddine
17:20-17:40		CHIKHI Sara	17:20-17:40		SAADIYA Benatmane
17:40-18:00		ZIANE Mohamed Issam	17:40-18:00		KHARCHI Nadia

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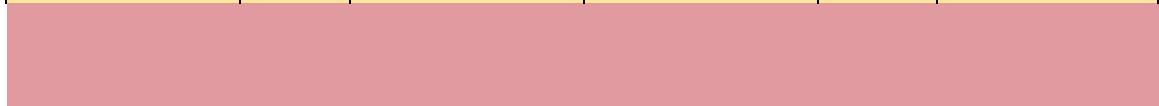
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09:30-10:00		Pr.Haddad Salim			
10:00-10:30		Pr.Bouzred Hamoudi			
		Pr.Maazouzi Ismaïne			
Time		room1	Time	Code	room2
10:30-11:00		BOUDJEDAA Tahar			BENAISSA Amina
11:00-11:20		BENHACHEM F,Zahra	11:00-11:20		HOUDA Amina

11:20-11:40		OTMANI Sadok	11:20-11:40		AOUICI Samia
11:40-12:00		Walid younsi	11:40-12:00		DJEGHLOUL F,Zohra
12:00-13:00	Coffee break		Coffee break	Coffee break	
		Chairman			Chairman
Time		room1	Time	Code	Room2
13:00-13:20		BENKHANOUCHE Zoubir	13:00-13:20		KEHAL Youcef
13:20-13:40		MESSAI Ridha	13:20-13:40		KEHAL Abir
13:40-14:00		KEBAILI Selwa	13:40-14:00		MOURES Nadjiba
14:00-14:20		HARIDI Ryad	14:00-14:20		CHERIET Loubna
14:20-14:40			14:20-14:40		TAGUIDA Nesrine

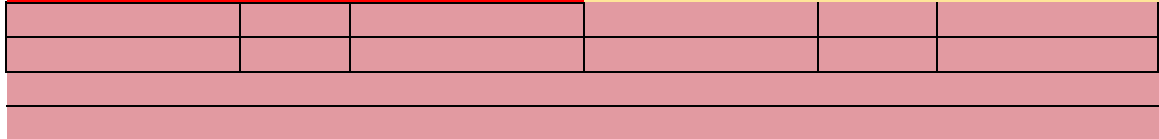
		Chairman			Chairman
Time		Online1	Time	Code	Online2
17:00-17:20		BENAKCHA Mansoura	17:00-17:20		SAADIYA Benatmane
17:20-17:40		LAKRI Amel	17:20-17:40		Djilali Khadidja
17:40-18:00		HANNACHI Ibtissem	17:40-18:00		



Coffee break		Coffee break		Coffee break	
Time	Code	Chairman Room3	Time	Code	Chairman Room 4
13:00-13:20		LAOUEZ Nadjat	13:00-13:20		ZAIEM Slimane
13:20-13:40		BEGAG Abdelaziz	13:20-13:40		BENHACHEM Fatim
13:40-14:00		LAOUER Abdelghani	13:40-14:00		SID-SAHTOUT Nazil
14:00-14:20		BOUADI Abdelkader	14:00-14:20		MENASRI Abdellah
14:20-14:40		REZIG Walid	14:20-14:40		



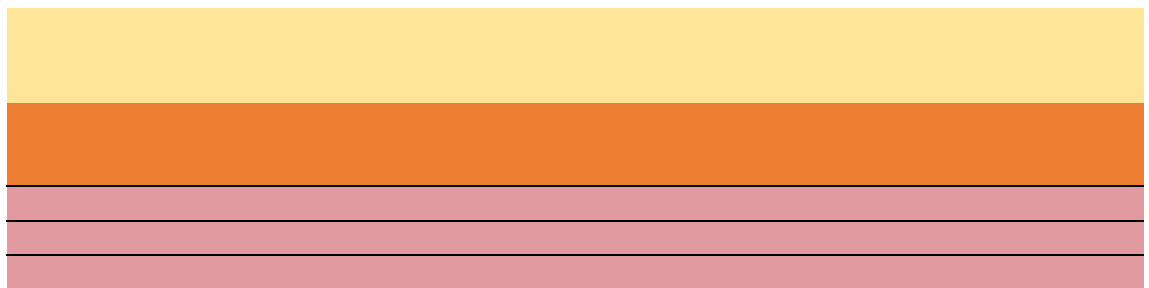
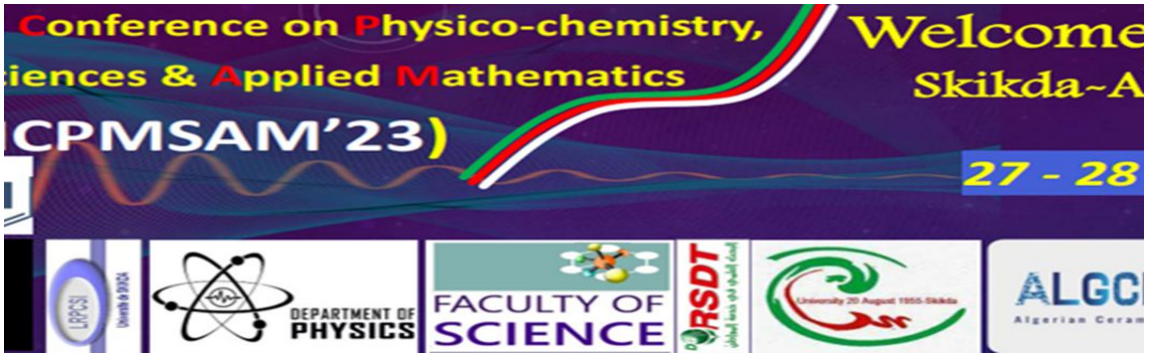
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17:00-17:20		SLATNIA Randa
17:20-17:40		ABDELDJEBAR Hasnia
17:40-18:00		MEDJANE Chahinez



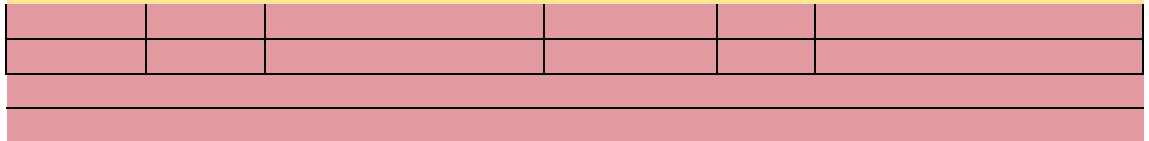
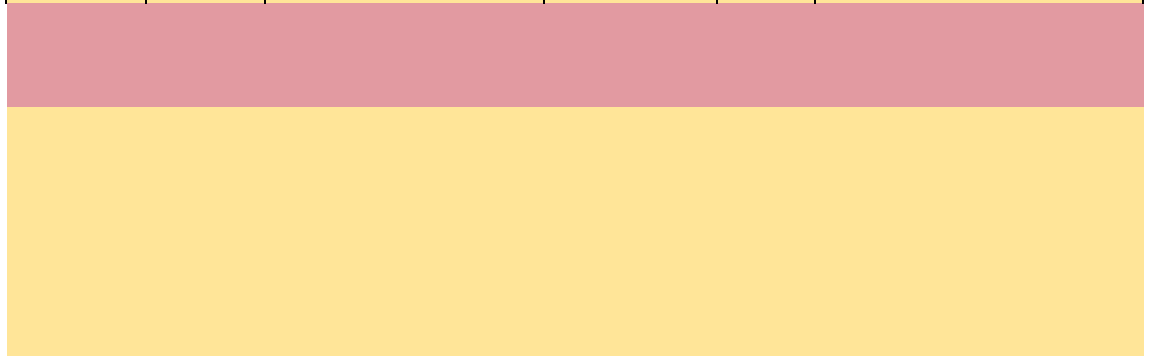
Time	Code	room3	Time	Code	room 4
10:30-11:00		MERAD Mahmoud	10:30-11:00		Grimed HOURIA
11:00-11:20		ROULA Abdelmalek	11:00-11:20		Ketfi M. El Amine

11:20-11:40		O. Chahaoui	11:20-11:40		BOULECHFAR Rahim
11:40-12:00		ZERGANE Said	11:40-12:00		
Coffee break		Coffee break		Coffee break	
		Chairman			Chairman
Time	Code	Room3	Time	Code	Room 4
13:00-13:20		SENOUCI Yasmine	13:00-13:20		BENABDELLAZIZ Ou
13:20-13:40		BOUSLAH Zineb	13:20-13:40		HANNACHI Ibtissem
13:40-14:00		BOUGHEZALA Nasrin	13:40-14:00		MOKRANI Khawla
14:00-14:20		BENKHANOUCHE.Z	14:00-14:20		CHEBLI Fatiha
14:20-14:40		MALAOUI Yousra	14:20-14:40		KERBICHE Hind

		Chairman
Time	Code	Online 3
17:00-17:20		
17:20-17:40		
17:40-18:00		



Coffee break Coffee break					
Time	Code	Chairman	Room 5		
13:00-13:20		CHERAITIA Abdallah			
13:20-13:40		BOULAHROUZ Salim			
13:40-14:00		BABOURI Kaoutar			
14:00-14:20		MOSBAH Salima			
14:20-14:40					



Time	Code	room 5	Time	Code	Online
10:30-11:00					
11:00-11:20					

11:20-11:40					
11:40-12:00					
Coffee break Coffee break					
		Chairman			
Time	Code	Room 5	Time	Code	Online
13:00-13:20		BABOURI Kaoutar	13:00-13:20		
13:20-13:40		BOUNIB Meriem	13:20-13:40		
13:40-14:00		KHALED Fatma Zohra	13:40-14:00		
14:00-14:20			14:00-14:20		
14:20-14:40			14:20-14:40		



Time	Code	Online

Time	Code	Online
13:00-13:20		
13:20-13:40		
13:40-14:00		
14:00-14:20		
14:20-14:40		