



Dipartimento di Fisica
Direttore: Prof. Michele Saba

CALL FOR RESEARCH FELLOWSHIP N. 5/2025 – REP. 76/2025 March 06, 2025

Title: “Theoretical and Computational Study of Alloyed Semiconductor Oxides and Green Organic Perovskites for Power Electronics and Solar Cells” - Scientific Manager: prof. Giancarlo Cappellini

THE DIRECTOR

Having considered Law nr. 240, December 30, 2010, assessing “Regulations for the organization of the Universities, of the academic staff and their recruitment and delegating to the Government the enhancement of quality and efficiency of the University system”, and the art. 18, co.5, lett. f;

Having considered Law nr. 35, April 4, 2012, which converted into law the Decree Law nr. 5, February 9, 2012, with amendments, containing urgent provisions on the simplification and development, in particular the art. 49, comma 1, lett. h, which amended the Art. nr. 18, co.5, lett. F, Law nr. 240, December 30, 2010;

Having considered D.lgs. nr. 196, June 30, 2003, “Personal Data Protection Code”, as modified by d.lgs. nr.101, August 10, 2018, establishing procedures to adapt the national law provisions for the adaptation of national law to the General Data Protection Regulation (EU) 2016/679 (GDPR), on data protection and privacy

Having considered D.lgs. nr. 82, March 7, 2005, “Digital Administration Code“, as amended;

Having considered D.lgs. nr. 198, April 11, 2006, "Code of equal opportunities between men and women" as amended;

Having regard to D.P.R. nr. 189, July 30, 2009, in particular the Art.2, "Recognition of foreign qualifications for access to public competitions";

Having considered the University Statute issued by D.R. nr. 339, March 27, 2012, lastly amended by D.R. nr. 305, March 28, 2022;

Having considered the University Regulation about research grants, last amended by D.R. no. 432, June 13, 2018;

Having considered the research project “ICT and Industry 4.0 technologies for the analysis and engineering of complex food systems for the production of local artisanal breads with high added value (AISAC)”, financed by Ministero delle Imprese e del Made in Italy (MIMIT); - CUP B29J23001120005”, Principal Investigator prof. Giancarlo Cappellini;

Having considered Prof. Cappellini’s request of a selection procedure for the assignment of nr. 1 research grant, with a duration of 6 (six) months, and a gross of legal charges under the Italian Tax amount of € 9000,00 (nine thousand euros) entitled “Theoretical and Computational Study of Alloyed Semiconductor Oxides and Green Organic Perovskites for Power Electronics and Solar Cells”– scientific manager prof. Giancarlo Cappellini, financed by Ministero delle Imprese e del Made in Italy (MIMIT); - CUP B29J23001120005”, Principal Investigator prof. Giancarlo Cappellini;

Having considered the resolution of the Department Council, report nr.2/2025 – February 20, 2025, which



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approved the request made by prof. Cappellini;

Having considered D.lgs. nr. 33, March 14, 2013, "Reorganization of the regulations concerning the obligations of publicity, transparency and dissemination of information by the Public Administrations" as amended;

Ascertained the availability of funds to cover the fellowships on the project RICALTRO_WP_CTC_2023_AISAC_PERSONALE_FANTI

HEREBY DECREES

ARTICLE ONE

(Characteristics of the project programme)

A selection, based on qualifications and interview, has been published to assign the fellowship with the following characteristics:

Funding Authority: Ministero delle Imprese e del Made in Italy (MIMIT)

Project deadline: January 01, 2027

Place for the implementation of the research: Department of Physics – University of Cagliari

Scientific Manager: Giancarlo Cappellini

Fellowship number: 1

Fellowship duration: 6 months

Annual gross amount: € 9000,00

Title of the project (Italian): “Studio teorico-computazionale di leghe a base di ossidi semiconduttori con ampio band-gap e perovskiti organiche verdi per elettronica di potenza e celle solari”

Brief description of the project (Italian):

Una delle attuali frontiere della ricerca sui semiconduttori è lo sviluppo di nuovi materiali che riducano al minimo l’impatto ambientale e soddisfino le esigenze di generazione e distribuzione dell’energia. Centrali elettriche piccole e più efficienti stanno sostituendo gli impianti su larga scala, concentrandosi sui dispositivi di conversione dell’energia solare. In questo contesto, due classi di materiali sono emerse come candidati importanti: le leghe di semiconduttori per l’elettronica di potenza e celle solari prive di metalli pesanti come alternative ai dispositivi a base di silicio.

Questo progetto teorico-computazionale vuole indagare le proprietà elettroniche e termodinamiche delle leghe di semiconduttori a banda larga e ultralarga (WBG eUWBG) - In_2O_3 e Ga_2O_3 - per applicazioni nell’elettronica di potenza, nonché le proprietà elettroniche della perovskite MASnI_3 , in cui il cesio è sostituito dal metilammonio (MA). Le leghe In_2O_3 - Ga_2O_3 mostrano valori di band-gap che vanno da 3,1 a 4,6 eV e un’elevata modificabilità delle proprietà elettroniche ed ottiche, rendendole promettenti per l’elettronica di potenza e l’optoelettronica.

Le sfide principali in questo tipo di ricerca includono le correzioni di quasi-particella per descrivere accuratamente le proprietà elettroniche. Per le leghe, una delle maggiori difficoltà risiede anche nella mancanza di metodi termodinamici rigorosi, mentre il MASnI_3 soffre di elevati tassi di degradazione. Le sfide principali in questo tipo di ricerca includono correzioni di quasi-particella (self-energia) per



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descrivere accuratamente le proprietà elettroniche, poiché la teoria del funzionale della densità (DFT) tipicamente sottostima il band-gap. Questo progetto di studio vuole utilizzare metodi DFT-1/2, che sono meno costosi dal punto di vista computazionale rispetto ai funzionali ibridi e agli approcci GW, insieme a nuove tecniche per la termodinamica delle leghe.

Verranno inoltre affrontati gli effetti eccitonici (effetti a due particelle) in differenti approssimazioni.

L'obiettivo è studiare come il drogaggio di MASnI_3 con Ba^{2+} , Ca^{2+} o Ge^{2+} , influisce sulla stabilità del composto. Allo stesso modo, per $\text{In}_x\text{Ga}_{1-x}\text{O}_3$, miriamo ad analizzare le sue proprietà elettroniche e termodinamiche per supportare strategie di ingegneria dei materiali per la stabilità strutturale.

Title of the project (English): “Theoretical and Computational Study of Alloyed Semiconductor Oxides and Green Organic Perovskites for Power Electronics and Solar Cells”

Brief description of the project (English):

One of the current frontiers in semiconductor research is the development of new materials that minimize environmental impact and meet the demands of energy generation and distribution. Small, more efficient power plants are replacing large-scale facilities, with a focus on solar energy conversion devices. In this context, two classes of materials have emerged as prominent candidates: semiconductor alloys for power electronics and heavy-metal-free solar cells as alternatives to silicon-based devices.

This theoretical-computational project investigates the electronic and thermodynamic properties of wide and ultrawide bandgap (WBG and UWBG) semiconductor alloys— In_2O_3 and Ga_2O_3 —for applications in power electronics, as well as the electronic properties of the perovskite MASnI_3 , in which cesium is replaced by methylammonium (MA). In_2O_3 - Ga_2O_3 alloys exhibit bandgaps ranging from 3.1 to 4.6 eV and high tunability of electronic and optical properties, making them

promising for power electronics and optoelectronics. Meanwhile, MASnI_3 , with a bandgap of 1.3 to 1.4 eV, high optical absorption, and excellent charge carrier mobility, is a strong candidate for solar cell applications.

Key challenges in this type of research include quasiparticles (self-energy) corrections to accurately describe electronic properties, as density functional theory (DFT) underestimates the bandgap. For alloys, a major difficulty also lies in the lack of rigorous thermodynamic methods, while MASnI_3 suffers from high degradation rates. This study employs DFT-1/2 methods, which are computationally less expensive than hybrid functionals and GW approaches, along with new the chemical techniques for alloy thermodynamics. Excitonic (two-particle effects) will be also addressed within different approximations.

The objective is to investigate how doping MASnI_3 with Ba^{2+} , Ca^{2+} , or Ge^{2+} —elements that theoretically mitigate Sn^{2+} oxidation—affects its stability. Similarly, for $\text{In}_x\text{Ga}_{1-x}\text{O}_3$, we aim to analyze its electronic and thermodynamic properties to support material engineering strategies for structural stability.



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ARTICLE TWO (Admission requirements, incompatibility, and duration)

Admission to the selection is open to graduates, regardless of nationality, holding (ref. to the Italian university system):

- A) A degree awarded according to the Italian Ministerial Decree nr. 270/2004 (laurea magistrale) in Physics, Electrical Engineering or Electronic Engineering;
- B) Proven experience in theoretical-computational studies on quasi-particle (self-energy) electronic and excitonic effects in oxides.

Validity and equivalence of degrees issued by foreign Universities must be assessed, in terms of duration, level of degree and fields of study in comparison to the degree listed above, and providing access to PhD education in the awarding country. The Selection Board will deliberate on its equivalence, in compliance with the current legislation in Italy and in the Country where it was issued, and within the framework of the international treaties or agreements concerning the recognition of qualifications for further studies for the sole purpose of the admission to the selection.

Additional evaluable qualifications (total score 60/100):

- A) Scientific publications on related subjects, up to 20 points;
- B) PhD in Physics on related subjects, up to 20 points;
- C) Experiences inherent to the research project, up to 20 points.

The entry qualifications must be held by the deadline established for the submission of the applications to the selection.

Applicants will not be admitted to the selection if not awarding any of the entry qualifications mentioned above by the deadline given for the presentation of applications to the selection, and, additionally, if applicants fulfil one of the following criteria:

- a) Public permanent employees in universities, in institutions and public centres for research;
- b) Relatives by blood and marriage, within the fourth degree, with staff members of the proposing Department, or with the Rector, the General Manager, or with a member of the Board of Directors at the University (Art. 18, par. 1, lett. B and c, law 240/2010);
- c) if they have had any other relations with the University of Cagliari, or with other Universities, or with the authorities included in the art. 22, par. 1 of the law 240/2010, as researchers for fixed terms in accordance with the art. 24 of the L. 240/2010, and as grant holders according to the art. 22 of the law 240/2010, for more than twelve years, summing up the duration of the grant awarded in this call. The periods spent off work for pregnancy or for health problems will not be taken into account (par. 9, art. 22, law 240/2010).

The applicant is accepted to the selection conditionally; failing these qualifications, the Director can decide at any time, through a motivated decision, to reject the application.



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The fellowship is not compatible with:

- a) Other fellowships awarded for any reason, with the exception of those granted by national or foreign institutions useful for integrating the research activity of the fellowship's holder during abroad periods;
 - b) The attendance to research doctorate courses with fellowship and medical specialization, in Italy and abroad;
 - c) Research grants;
 - d) Employment relationships, without prejudice to the possibility that the fellowships holder may be placed on unpaid leave;
 - e) Self-employment activity, even para-subordinate, with the exceptions listed in the following paragraph;
- 2 – The fellow may carry out occasional self-employment activities, even semi-subordinate, upon written communication to the Scientific Manager and on condition that:
- a) This activity is declared by the Scientific Manager compatible with the research activity presented in the Research Grant,
 - b) It does not involve a conflict of interest with the specific research activity carried out by the fellow
 - c) Do not harm the University, in relation to the activities carried out.

ARTICLE THREE

(Applications)

Applications to the selection (form Annex A) and all the requested documentation, including the publications, must be submitted in PDF (portable document format) via certified mail (PEC) to protocollo@pec.unica.it within the 20th day starting from the day following the date of publication on the UNICA "Laureati" and "Department of Physics" websites. The subject must contain:

DIP. PHYSICS - Research grant N. 5/2025 - Scientific manager: prof. Giancarlo Cappellini

The application form and the other documents that need to be signed will be signed by Digital Signature or handwritten signature.

The university administration will verify all the self-certifications according to T.U. 445/2000.

All communications between the office and the applicants will be forwarded only by PEC or e-mail. Applications and qualifications submitted after the deadline established for the presentation of applications to the selection will not be considered.

The university administration is not responsible for the lost of applications or related documents if this is due to incorrect contact details provided by the applicant or having failed or delayed in notifying any changes of the contact details, nor for any possible misdelivery or telegraph error.

The applicant must include in the application:

- a) substitutive declaration of certifications, issued pursuant to the D.P.R. 445 – 12.28.2000, relating to the candidate's educational, didactic, scientific, and professional curriculum (Annex B)



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- b) substitutive declaration of certifications, issued pursuant to the D.P.R. 445 – 12.28.2000, relating to the possession of additional evaluable qualifications, certifications, and work experiences, detailed in English or in Italian, drawn up according to the format in Annex C
- d) publications with attached declaration certifying compliance with the original (Annex D), issued pursuant to the D.P.R. 445 – 12.28.2000;
- e) if the qualifications required for admission were obtained abroad, a copy of the statement of recognition attesting their validity in Italy. In the event that the recognition has not yet been made, the equivalence will be assessed, solely for the purpose of admitting the candidate to the selection, by the Selection Committee;
- f) remote interview request form (Annex E) filled with all the requested information;
- g) two-sided coloured scanned copy of a valid ID, with a clear photo
- h) list of the documents and qualifications presented as attachments to the application.

ARTICLE FOUR
(Selection Committee)

The Selection Committee will be appointed by Director of Department's decree pursuant to the Art. nr. 5 of the University regulation and is composed of three experienced members, one of which acting as chairman, all chosen according to principles of equal opportunities, transparency and impartiality. The Committee is composed of:

- the Principal Investigator of the project
- two staff members from the same Macro–area Section or, if not available, from the same Area of the research project,

The Selection Committee can also be supplemented by one or more members designated by the funding entity as experts.

The selection ranking will be based on the qualifications and the interviews of the candidates, according to internationally recognized standards.

In the first session, the Selection Committee determines the evaluation criteria and the minimum score for being admitted to the interview. The applicants' ranking by the Committee will be in percent.

The Committee has 100 points totally, partitioned as follows:

- up to a maximum of 60/100 for the qualifications;
- up to a maximum of 40/100 for the interview.

The outcome of the assessment with its score, the possible admission to the interview, date and time of the interview, and the information on the procedures for carrying it out, will be published on the websites of Department of Physics and of University of Cagliari (unica.it) 15 days in advance.

The applicants will be included in the general ranked list on a decreasing order based on the total final score, obtained by adding qualification and interview scores. In case of further parity, the younger applicant will prevail.



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ARTICLE FIVE

(Awarding of the research fellowship, start and end of the activity)

After checking the selection documents and certifying the correctness of the Selection Committee's work, the general ranked list is approved by Director of Department's Decree and published on the University website.

The start of the activity will have to be certified providing a declaration of start research activity issued by the Principal Investigator to the Director of Department.

The fellow will carry out the project under the direct responsibility of the Principal Investigator of the project the fellowship has been awarded for. The fellow will be asked to issue an activity report at the end of the research period, that will be evaluated by the Principal Investigator. The fellow will work on the project in the Department associated with the Principal Investigator, using any equipment and service available in it. Upon Principal Investigator's permission, the project can be carried out also in other research facilities of the University, in qualified structures and/or in Italian or foreign centres.

The fellow must comply with the obligation of confidentiality in relation to the information, news, documents and knowledge acquired during her/his activity.

The fellow must stipulate an adequate compulsory personal insurance policy both against the risk of accidents occurring during the period of presence in the University structures, or at external structures that can host the fellow upon Principal Investigator's agreement. The insurance policy should also cover civil liability towards third parties, possibly deriving from damage to persons or things. A copy of the policy must be delivered to the administration on the starting date of the research activities at the Department of reference.

The fellowship will be paid in monthly postponed instalments.

The fellow's activity must be completed by the expiry date of the research project.

The success of the research grant does not determine the establishment of an employment relationship, does not give rise to social security treatments, to evaluations for the purposes of legal and economic careers, nor to automatic recognitions for social security purposes.

ARTICLE SIX

(Personal data processing)

The University of Cagliari is responsible for the treatment of personal data according to the General Data Protection Regulation (GDPR) (EU) 2016/679, and the Personal Data Protection Code – Leg. Decree n. 196 of 30 June 2003, in respect of subjects' rights, fundamental freedoms and dignity. Privacy policy for the category of Citizens is published on the following website: https://www.unica.it/unica/it/utility_privacy.pag

According to Art. nr. 5 of the Law nr. 241, August 7, 1990, the management of the selection procedures related to this call is attributed to dr. Fernanda Marongiu, Administrative Manager of Department of Physics.

Candidates can exercise the right of access to the documents of the selection procedure according to the procedures set out in the D.P.R. 184 of 12.4.2006 (Regulation governing access to administrative documents).



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ARTICLE SEVEN

(Advertising and safety regulations)

The current call will be published on the web site of the University, (https://www.unica.it/unica/it/laureati_s07_ss01.page).

For what not explicitly mentioned in this announcement the University shall act in compliance with the rules included in the Law nr.240/2010 and under the regulations of the awarding of research grants in this University.

The Director of Department of Physics

Prof. Michele Saba

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