S16 Energy and Sustainability
Energía y Sostenibilidad (GEE)

12/07 Tuesday afternoon, Aula 1.6

15:30-16:10 Víctor A. de la Peña O'Shea (Instituto IMDEA Energia)
Solar fuels by artificial photosynthesis: from inorganic to hybrid multifunctional materials

16:10-16:30 Judit García Ferrero (Universidad de Salamanca)
Brayton cycle coupled to CSP plants: comparative analysis of central tower and parabolic dish farms

16:30-16:50 Francisco Cuadros Blázquez (Universidad de Extremadura)
Secuestro de Carbono en una Planta Híbrida Biogás-Fotovoltaica Seguida de un Proceso de Compostaje

17:00-18:00 **Posters and Coffee**

18:00-18:40 Mercedes Ballesteros Perdices (CIEMAT)
Aportaciones desde el sector energético a la lucha contra el cambio climático

18:40:19:00 Alberto Sánchez González (Universidad Carlos III)
Flux mapping in heliostat fields: Analytic function with astigmatism and defocus

19:00-19:20 Youssouf Doumbia (Universitat Politécnica de València)
Investigation of the stability and efficiency of MA-doped FAPbBr3 thin film for solar cells

Posters:

15 Pablo Palacios Clemente (Universidad Politécnica de Madrid, Instituto de Energía Solar)
Assessing composition engineering as mechanism to deal with stability and toxicity problems of inorganic halide perovskites with improved absorption features for photovoltaic applications

16 Antonio Angel Moya Molina (Universidad de Jaen)
Charge and energy stored in electric double layer capacitors from potentiostatic discharge

17 Victoria Beltran (Universidad Politécnica de Cartagena)
Artificial Intelligence Applied to the Prediction of Module Temperature for Building-Integrated Photovoltaic

S16 Energy and Sustainability
Energía y Sostenibilidad (GEE)

13/07 Wednesday afternoon, Aula 1.6

15:30-16:10 Carlos del Cañizo Nadal (Instituto de Energía Solar, Universidad Politécnica de Madrid)
Improving the quality of solar grade silicon through defect engineering

16:10-16:30 Joeluis Cerutti Torres (Universidad Politécnica de Madrid)
Into an accurate and low computational cost prediction of bandgaps in Copper based delafossite oxides: a DFT and ML study with experimental comparison

16:30-16:50 Klègayéré Emmanuel Koné (Universitat Politécnica de València)
Insight of ZnO/CuO and ZnO/Cu2O solar cells efficiency with SCAPS simulator

17:00-18:00 **Coffee Break**

18:00-18:20 Amal Bouich (Universitat Politécnica de València)
Opportunities and Challenges of Lead-Free Perovskite for high efficiency and stable solar cells with a low-cost technique

18:20-18:40 Armel Ignace N'Guessan (Universitat Politécnica de València)
Enhanced the CIGS solar cell efficiency through structural engineering at the buffer/CIGS interface

18:40-19:00 Pablo Sanchez Palencia Vallejo (Instituto de Energia Solar, Universidad Politécnica de Madrid)
The compositional and configurational space of spinel nitride solid solutions: accelerated exploration of electronic properties through machine learning

19:00-19-20 Roberto Gómez-Calvet (Universidad Europea de Valencia)
The 2030 power sector transition in Spain: advantages and drawbacks of massive deployment of solar photovoltaic sources

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Solar fuels by artificial photosynthesis: from inorganic to hybrid multifunctional materials

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The continuing rise in atmospheric CO_2 levels has become one of the most enduring problems faced by humankind. Finding sustainable ways to turn CO_2 into valuable products is imperative to mitigate global warming and to provide a long-term solution to the growing energy demand. Solar energy is the largest exploitable renewable energy source. By mimicking nature, the scientific community has devoted great efforts to develop different technologies such as artificial photosynthesis (AP), where solar energy and natural resources can be directly converted into renewable and carbon-neutral fuels and chemicals.

Photocatalytic materials have focused on the use of inorganic semiconductors such as metal oxides and chalcogenides. In this work, different strategies to modulate the light response and improve the charge separation and transport such as: (i) The modification of optoelectronic properties of through the use of band gap engineering strategies, allow controlling the absorption of incident photons, redox capabilities and subsequently the photocatalytic performance; (ii) the use of co-catalysts play an important role in the selectivity; (iii) the design of multijuntions materials such as hybrid composed by a mixture of inorganic and organic semiconductors. In the case of organic one, the development of conjugated porous polymers have recently attracted significant attention as promising photocatalysts for solar fuel generation. The synergy between organic and inorganic semiconductors results in an extended light absorption range, improved textural properties and higher stability to photo-corrosion. Interestingly, these hybrid heterostructures can effectively facilitate the charge transfer and reduce the recombination of photogenerated electrons and holes, resulting in enhanced photocatalytic performances.

A deeper understanding of the reaction mechanism is crucial to achieve real progress in the development of the AP process, directly impacting on the advance of solar fuels technologies and multitude of light-driven reactions. However, this is a complex issue that involves multielectronic reactions occurring at different timescales (i.e. fs-s). In order to clarify the effect of different parallel and competitive reactions in the activity and products distribution, advanced in-situ characterization and theoretical calculations were performed to clarify the reaction mechanism of these systems.

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Brayton cycle coupled to CSP plants: comparative analysis of central tower and parabolic dish farms

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Solar energy is one of the most promising alternative energy sources. Particularly, Concentrated Solar Power (CSP) technology has the potential to provide not only electrical but also thermal energy. CSP systems are highly flexible to be configurated in multiple ways: hybridized with fuel (conventional or renewable) for dispatchable generation, coupled with thermal energy storage or even hybridized with other renewable energy systems as PV.

Two different Concentrated Solar Power (CSP) technologies are analyzed from a thermodynamic and thermo-economic perspective. A Central Solar Tower (ST) plant and an array of Parabolic Dishes (PD) performing a single-stage recuperative Brayton cycle are compared for two power outputs (4.6 MW and 20 MW) and different locations placed approximately at the same longitude and quite different latitudes in a south-north line: Ouarzazate (Morocco), Seville and Salamanca (both in Spain). While the ST counts with a Brayton cycle turbine in the range of MW, each PD that compounds the farm integrates a micro-gas turbine in other to achieve the power outputs mentioned above. The power block is hybridized with a combustion chamber aiming to supply energy under lack of solar irradiance conditions. The thermodynamic model for each system is further developed in previous works [1], including all the subsystem efficiencies and losses. Aiming to compare the two CSP systems from the thermo-economic viewpoint, a set of economic indicators such as the Levelized Cost of Electricity (LCoE), Net Present Value, Benefit to Cost Ratio and Internal Rate of Return are surveyed.

In regard of thermodynamics, some results should be pointed out. Among the locations studied, Ouarzazate presents the maximum solar records, yielding to the highest annual solar share, specially for 20 MW scale (0.54 for ST and 0.76 for PD). But it is important to note that overall plant thermal efficiency is greatly influenced by ambient temperatures. Thus, northern locations as Salamanca, with relatively poorer solar conditions, but with lower ambient temperatures, allow good overall efficiencies. For ST, overall and heat engine efficiencies overpass PD results by 35% for all the locations and power scales. Regarding thermo-economic indicators, Fig. 1 depicts the LCoE outputs obtained for all cases studied. The best LCoE is achieved by ST at 20 MW power scale in Ouarzazate (135 USD/MWh) and the worst result is presented by PD, 4.6 MW, in Salamanca (203.5 USD/ MWh). These values are in the range of other CSP projects including stand-alone PD and thermal storage ST geometries [2].

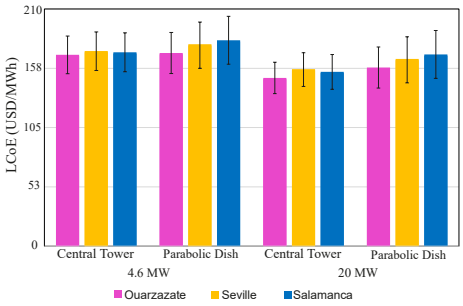

Figure 1: Levelized Cost of Electricity (LCoE) results for ST and PD technologies, three locations and two power scales (4.6 MW and 20 MW).

Although this study proves that this kind of technology is feasible and bankable, more research is needed in order to lower costs, reach economic indicators comparable to other renewable technologies, and promote a solid integration of CSP systems into the market.

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Secuestro de Carbono en una Planta Híbrida Biogás-Fotovoltaica Seguida de un Proceso de Compostaje

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Actualmente, en España el destino mayoritario de todos los residuos sólidos urbanos e industriales es el vertedero. Las otras vías de gestión posibles, mucho más recomendables desde el punto de vista energético y medioambiental, como son el reciclaje o la valorización material o energética, si bien han ido aumentando su implantación en los últimos años, representan aún unos niveles muy por debajo de la media de la Unión Europea. Concretamente, el 24,32% en España frente al 36% de media en Europa [1], [2].

En regiones como Extremadura, donde el peso del sector agroindustial es muy importante, es necesaria la implantación de tecnologías biológicas de tratamiento de los residuos que generan, ya que contienen un alto poder contaminante. En efecto, varios estudios realizados previamente por el Grupo de Investigación DTERMA de la Universidad de Extremadura (al cual pertenecen dos de los autores de la presente comunicación) indican que la contaminación anual producida solo por las industrias almazarera, vitivinícola, tomatera y de matadero de cerdos es equivalente a la generada anualmente por la población residente en nuestra región.

Dicho Grupo de Investigación ha publicado varios trabajos sobre la viabilidad energética, económica y medioambiental de la Biometanización (o Digestión Anaerobia, DA) de los residuos agroindustriales en Extremadura, cuantificando el secuestro de carbono provocado en dicho proceso (ver, por ejemplo, [3]) Sin embargo, el contenido de carbono del residuo tratado mediante DA no se acaba aquí, es necesario enlazar a continuación con un proceso de compostaje del digestato (fracción sólida del efluente obtenido tras la DA), de modo que se cierre el ciclo ecológico completo del carbono "desde la cuna hasta la tumba".

En este trabajo se presentan los resultados obtenidos sobre el secuestro de carbono obtenido en la codigestión de un 90 % de residuos de la industria láctea (lactosuero) y de un 10% de estiércol de oveja llevada a cabo en una planta piloto de unos 2 m^3 de capacidad del biodigestor, alimentada eléctricamente con una instalación fotovoltaica de unos 0,5 kWp. Después de la DA se ha continuado con el compostaje de la fracción sólida del efluente digerido (40% del total), hasta obtener un enmendante agrícola de gran calidad. La fracción líquida (el 60% restante) se ha analizado y se ha comprobado que es apta para su uso en riego de frutales cuyo fruto no entre en contacto con ella o en riego de forrajes para alimentación animal, cerrando así el ciclo de vida del residuo inicial.

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Aportaciones desde el sector energético a la lucha contra el cambio climático

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Los esfuerzos mundiales realizados, hasta la fecha, para mitigar el cambio climático culminaron en el Acuerdo de París de 2015, en virtud del cual 195 países adoptaron el primer acuerdo, universal y vinculante jurídicamente, para mantener el incremento de la temperatura media mundial por debajo de 2 °C y seguir esforzándose por limitar el aumento a 1,5 °C. Este objetivo climático es tremendamente ambicioso y, teniendo en cuenta que la producción de electricidad y el transporte son responsables del 70% de las emisiones de gases de efecto invernadero [1], no podrá alcanzarse sin una reforma importante de los sistemas de producción y consumo de energía a escala mundial.

Existe consenso a nivel mundial en considerar que el modelo energético actual, basado en el crecimiento del consumo y en el uso de recursos fósiles, es insostenible, tanto por los riesgos relativos a la seguridad de suministro como por su contribución al cambio climático. La UE, comprometida con los Acuerdos de París, ha considerado que la descarbonización del sector de la energía constituye un paso crucial para la neutralidad climática de la UE y por ello, a finales del 2018 el Consejo europeo aprobó el denominado Paquete de Energía Limpia para todos los europeos (también conocido como "paquete de invierno") [2], orientado a alcanzar los objetivos climáticos europeos a 2030 (al menos 55% de reducción), manteniendo la seguridad de suministro y la competitividad de los precios de la energía.

Para cumplir estos objetivos, el reglamento de gobernanza establece que todos los Estados miembros deben elaborar su Plan Nacional Integrado de Energía y Clima (PNIEC) para el período de 2021 a 2030. Los PNIECs, además de fijar los objetivos de reducción de emisiones de gases de efecto invernadero y de penetración de renovables y eficiencia y ahorro energético, incluyen objetivos nacionales de financiación, así como objetivos para implementar tecnologías bajas en carbono en 2050.

El PNIEC español fue aprobado por el Consejo de Ministros el 16 de marzo de 2021 y publicado en el BOE de marzo del mismo año [3]. El PNIEC identifica objetivos y adopta medidas en las cinco dimensiones de la Unión de la Energía: la descarbonización, incluidas las energías renovables; la eficiencia energética; la seguridad energética; el mercado interior de la energía y la investigación, innovación y competitividad. Entre otras medidas, se prevé el impulso de la instalación de potencia de producción de origen renovable, cuya distribución concreta por tecnologías renovables dependerá de la evolución de los costes relativos de cada una de ellas; el cese total de la actividad de centrales de carbón como máximo en 2030; el impulso de las tecnologías de almacenamiento, así como del coche eléctrico y del uso de biocarburantes

En esta ponencia se presentará el conjunto de objetivos y compromisos de la Unión Europea para la descarbonización del sector energético y se analizan las principales características del PNIEC español.

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Flux mapping in heliostat fields: Analytic function with astigmatism and defocus

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Thousands of mirrors, called heliostats, track the sun and concentrate solar energy into a central receiver atop a tower in Solar Power Tower (SPT) plants. Sunray incidence on the mirror is not normal, leading to off-axis aberrations or astigmatism, that distort the flux distribution on the target [1]. This work presents a flux mapping model that reproduces the aberrations due to heliostat defocus and astigmatism.

There are two flux mapping approaches: Monte Carlo Ray-Tracing (MCRT) and convolution. The convolution method, faster than MCRT, produces analytic functions from the superposition of error cones (concentration, sunshape, and optical errors). However, the existing analytic functions disregard the effect of astigmatism, which is relevant in actual plants.

Depending on the defocus distance from the circle of least confusion (δ), Igel and Hughes [2] stated the geometric relationships between tangential and sagittal planes. These correlations have been introduced in UNIZAR analytic function [3], which is valid for unusual, focused heliostats ($\delta = 0$).

The following proposed analytic function computes the concentration ratio of flux density (C) as a function of ξ and ζ, heliostat coordinates on the image plane, where *erf* stand for the Gaussian error function and *aw* and *ah* are the integration limits.

$$C = \frac{\cos\omega}{J} \cdot 0.25 \cdot [erf\,(\xi + aw) - erf\,(\xi - aw)] \cdot [erf\,(\zeta + ah) - erf\,(\zeta - ah)]$$

The proposed analytic function is validated against MCRT simulations. For instance, for incidence angle $\omega = 60°$, Figure 1 compares both flux maps for several δ defocus planes.

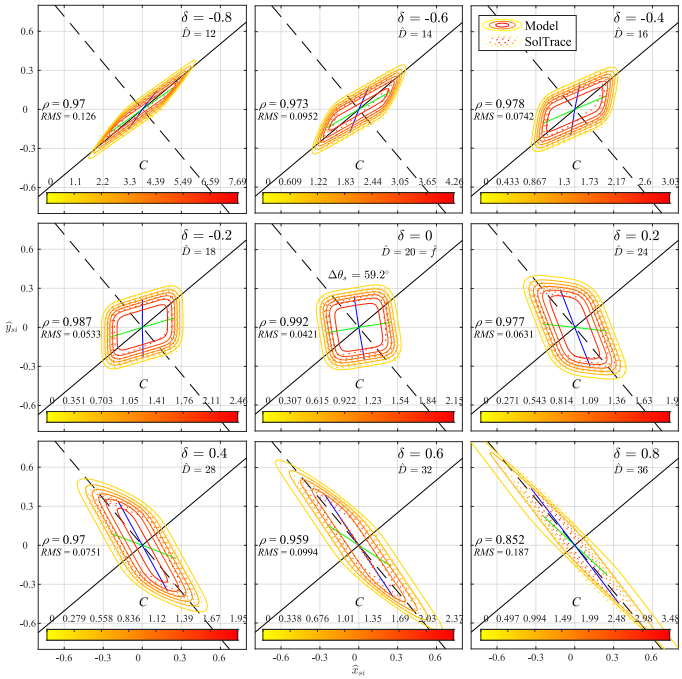

Figure 1. Concentration maps by the model (solid lines) and MCRT (dotted) for several δ defocus distances.

For Gemasolar plant, consisting of 2650 heliostat and a 18-panel cylindrical receiver, the following Figure 2 shows the flux map at 8:30 solar time in the Equinox.

In comparison with MCRT Cross-correlation coefficients above 90% are achieved with the proposed analytic function.

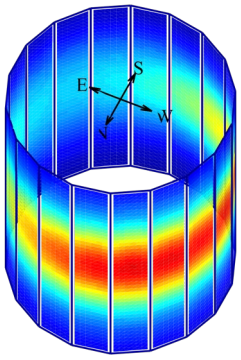

Figure 2. Flux map on receiver by Gemasolar heliostat field.

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Investigation of the stability and efficiency of MA-doped $FAPbBr_3$ thin film for solar cells

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Organometal halide perovskite solar cells are becoming one of the most competitive emerging technologies. They have achieved a power conversion efficiency (PCE) of 22.7% in 10 years. They generally have excellent efficiency but low stability. This degradation of perovskite devices has been associated with mobile ion migration. The $MAPbBr_3$ perovskite materials are significantly more stable under ambient conditions but have a more significant bandgap (2.3 eV) than the $FAPbBr_3$ perovskite materials, which are interesting bandgap. This work uses a mixture of these two materials with a high proportion of $FAPbBr_3$ to obtain a stable active layer with a suitable bandgap by the one-step spin-coating method. We used a ratio of 6% of MA in the mixture to prepare the layer. In addition, the prepared layer was annealed for 30 min at 100°C.

We found intermediate properties as expected, notably the stability and the bandgap, whose value is 1.93 eV. Indeed, the degradation process of the prepared thin film is slower than that of pure $FAPbBr_3$. The absorption of the mixture is suitable for use in photovoltaics.

Assessing composition engineering as mechanism to deal with stability and toxicity problems of inorganic halide perovskites with improved absorption features for photovoltaic applications.

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Inorganic perovskites like CsPbI3 are emerging as a family of very promising materials to be used in the photovoltaic field as absorber materials. Nevertheless, besides their remarkable optical absorption properties, these materials have encountered two important bumps in their road towards commercialization, their poor stability and toxicity, being caused the latter by their Pb content. In this work, we explore the possibility of lessening these two problems, as well as obtaining improved photovoltaic efficiencies, through the propitious fine-tuning of the chemical composition. For that purpose, we have performed a systematic DFT study of RbaCs1-aSnbPb1-bI2Br (a = 0 - 0.125, b = 0 -1) perovskites, studying in detail the effects of composition changes and related solid structure distortions on the optoelectronic properties of these materials. Our results provide a complete description on the connections between the chemical composition, crystal structure, intrinsic stability and electronic properties of these materials, which ultimately define their absorption features. Our results suggest that all-inorganic RbaCs1-aSnbPb1-bI2Br ($1 > b > 0.5$) perovskites meet all the requirements to be highlighted very adequate candidates for photovoltaic applications, thanks to their reduced content in Pb and their improved intrinsic stability and absorption features.

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Charge and energy stored in electric double layer capacitors from potentiostatic discharge

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Electric double layer (EDL) capacitors are electrochemical energy storage devices consisting of two activated carbon porous electrodes separated by liquid electrolyte with a salt dissolved in an aqueous or organic solvent. They store electric charge in the electric double layers at the electrolyte-electrode interfaces without the requirement of redox reactions. These devices show much higher specific energy than conventional capacitors due to high surface area of activated carbon porous electrodes. They, together with rechargeable batteries, store electric charges and therefore renewable energy in a fast, safe and efficient manner so they find application not only in portable electronic devices and electric vehicles, but also as a complement to fluctuating energy sources, such as wind and sunlight. Unlike rechargeable batteries, EDL capacitors present high specific power, rapid charge-discharge capability, and long cycle life.

Electrochemical characterization of EDL capacitors is a classic research topic in the field of the electrochemical power sources [1]. EDL capacitors are usually characterized, by analogy to conventional capacitors, by their differential capacitance. This capacitance can be experimentally determined by using different conventional electrochemical techniques such as cyclic voltammetry, electrochemical impedance spectroscopy, galvanostatic charge-discharge or potentiostatic charge-discharge through a resistor. The experimental data are then interpreted by using a simple electric circuit constituted by the series combination of the equivalent series resistance and the mentioned differential capacitance. In particular, charge and energy are determined from this capacitance by using the usual expressions in conventional capacitors. However, studies on the direct measurement of the electric charge stored in EDL capacitors from the time evolution of the electric current during the discharge through a resistor, have been rare in literature. This can be due to the high values reached by the initial electric current, as well as to the long experimentation time being necessary to obtain precise values of the charge.

In this work, we obtain the electric charge stored in an EDL capacitor from the potentiostatic discharge through a resistor without using an equivalent electric circuit model. Three commercial EDL capacitors with nominal capacitances in the range from 0.1 to 1 F, are selected. The time evolution of the electric current obtained during the potentiostatic discharge through a resistor nominally 10 Ω is gathered by using an Autolab PGSTAT204 potentiostat/galvanostat, and the electric charge is determined by means of coulometric techniques from the area of the current-time curves. Evolution with the initial electric potential of the charge stored in the EDL capacitors, as shown in Figure 1, is analysed and discussed. The capacitance and energy are also studied as a function of the electric potential by means of different statistical parameters.

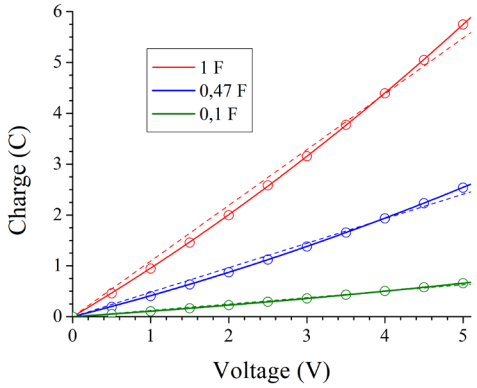

Figure 1. Evolution with potential of the electric charge stored in the EDL capacitors.

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Artificial Intelligence Applied to the Prediction of Module Temperature for Building-Integrated Photovoltaics

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Photovoltaic (PV) systems have been installed worldwide during last decays, reaching 894.2 GWp of installed capacity at the end of 2021 [1]. Building integrated photovoltaics (BIPV) configuration allows for producing electricity at the same place where it is going to be consumed, plus it helps expanding the PV areas for the decarbonization of the energy system [2]. Nevertheless, BIPV exhibits some disadvantages when comparing to ground mounted photovoltaics, such as poor air ventilation which could lead to high working temperatures. Controlling and predicting BIPV temperatures would help to better design the systems, calculate its potential production, as well as predict faults during its performance. Previous works have applied artificial intelligence (AI) techniques to predict module PV temperature, but always applied to ground-mounted PV systems.

The first study using artificial intelligence to model PV module temperature of a BIPV system was recently published [3], and its data is obtained from a deliberately designed set-up, called "PV-cubes" as described by Toledo et al. [4]. Grammatical and Differential evolution, which are classified as Genetic

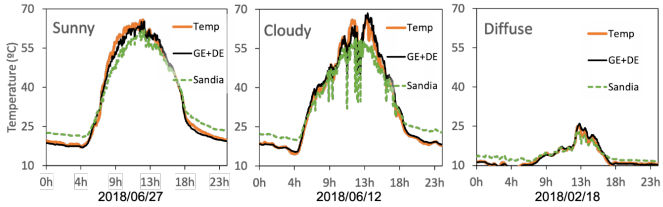

Figure 1. PV module temperature measured vs. modelled in three different types of days using two different approaches: the conventional Sandia model and Genetic Algorithms (Source: [3]).

Algorithms, were applied to 3 days dataset. Datasets were classified into three day-type groups: whether they belong to sunny, cloudy, or diffuse light-types days. The study obtained relative errors of less than 4% when predicting the module temperature. Figure 1 shows an example of the measured and predicted values of PV module temperature, as well as prediction using one of the most common PV module temperature models [5]. Here we present the Artificial Neural Network (ANN) method to predict the module temperature of BIPVs. We compare this method with the GE+DE algorithm and assess which of the two is the most reliable method to obtain a temperature predicting model.

[1] International Renewable Energy Agency (IRENA), Renewable Energy Statistics 2021, available on-line at: https://irena.org/publications/2021/Aug/Renewable-energy-statistics-2021

[2] T. E. Kuhn, C. Erban, M. Heinrich, J. Eisenlohr, F. Ensslen, and D. H. Neuhaus, Review of technological design options for building integrated photovoltaics (BIPV), *Energy and Buildings* **231**, 110381 (2021) doi: 10.1016/j.enbuild.2020.110381.

[3] L. Serrano-Luján, C. Toledo, J. M. Colmenar, J. Abad, and A. Urbina, Accurate thermal prediction model for building-integrated photovoltaics systems using guided artificial intelligence algorithms, *Applied Energy* **315**, 119015 (2022), doi: 10.1016/j.apenergy.2022.119015.

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Improving the quality of solar grade silicon through defect engineering

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A large fraction of the carbon footprint of a PV module comes from the silicon ultrapurification step. It takes 99% pure metallurgical silicon and ultrapurifies it to 99,9999999% or more, resulting in a product referred to as polysilicon, which is used to feed the crystal growers. The conventional purification process converts the metallurgical silicon to trichlorosilane, which is distilled and converted back to silicon in a Siemens-type reactor. A huge investment in electricity and cooling is needed, with energy demand in the range of 50-75 kWh/kg. Alternative purification routes that avoid the transformation to chlorosilanes by applying metallurgical-like methods are under research. The silicon feedstock produced this way, the so-called Upgraded Metallurgical Grade Silicon (UMG), besides being cheaper, requires less energy for its manufacture, in the range of 30 kWh/kg, resulting in a clear environmental benefit.

The challenge for UMG is to demonstrate that the electronic quality of the material is not ultimately limited by its purity, so that the beneficial impact "per kg" is also maintained as "per watt". In this respect, the presence of foreign elements and impurities in UMG-silicon in larger amounts than in standard polysilicon is at first sight a major handicap. However, a careful and precise mitigation of their eventual detrimental effects by means of impurity compensation and defect engineering carried out during the manufacturing process and the cell fabrication stage has demonstrated comparable levels of electronic quality between polysilicon and a novel UMG-Si developed by a Spanish company [1].

In this work, the quality of UMG-Si is characterized with a number of advanced techniques, including Photoconductance-based lifetime measurements. As an example, figure 1 shows carrier lifetime values after an optimized phosphorus diffusion gettering (PDG) process, reaching values higher than 200 µs for wafers coming from different ingots, bricks and heights in the brick. The possibility of implementing a second PDG process has also been studied, concluding that it is generally beneficial over a relatively wide range of experimental parameters, and that it allows to obtain a record value of 645 µs.

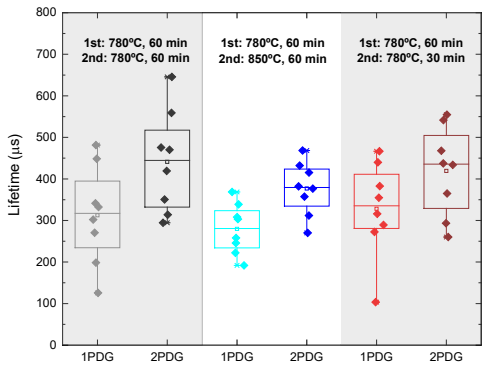

Figure 1. Lifetime values at 10^{15} cm^{-3} injection level obtained from UMG-Si wafers after PDG processes under the specified conditions.

These values are above the threshold value required to achieve >21% efficiency in state-of-the-art PERC solar cell structures [2].

In this work we will also explore a fabrication route for UMG-Si advanced solar cells, with the purpose of obtaining high-efficiency, low cost and more environmentally-friendly devices.

[1] E. Forniés *et al.*, *Solar Energy* **220**, 354 (2021).
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Acknowledgements: MCIN/ AEI /10.13039/501100011033 is acknowledged for funding the Project PID2020-113533RB-C31. This work is also part of the Project MADRID-PV2 (S2018/EMT-4308) funded by the Regional Government of Madrid with the support from FEDER Funds.

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Into an accurate and low computational cost prediction of bandgaps in Copper based delafossite oxides: a DFT and ML study with experimental comparison.

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Copper based delafossite oxides of the form $CuMO_2$ have been reported as promising candidates for transparent conducting oxides (TCOs) materials in the construction of solar cell devices, among other applications based on their optical and electronical properties [1]. We report density functional theory simulations on the compounds of the form $CuMO_2$ with $M = Al, Ga, Fe, Cr, Ni, Co$, and compare them with experimental results. For the calculations GGA, GGA+U and HSE schemes were tested, and their results compared. The use of hybrid functionals in HSE approximation improves considerably the bandgaps when compared with the experimental results but takes considerable time to converge. Therefore, using the projected DOS for the different elements in HSE simulations, different GGA+U were performed to obtain the parameter U that more accurately placed the d orbitals of the transition metals in the valence band. Having the bands accurately described in a GGA+U scheme, other optical calculations with a reasonable computational cost and an acceptable accuracy can be performed. Lastly, machine learning is used to estimate the bandgaps of mixed delafossite compounds of the form $CuM_xN_{1-x}O_2$ being M, N the same metals previously mentioned.

[1] H. Shaili *et al*, *RSC Adv.* **11**, 25686 (2021).

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Insight of ZnO/CuO and ZnO/Cu_2O solar cells efficiency with SCAPS simulator

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Despite the low power conversion efficiency of ZnO/CuO and ZnO/Cu_2O solar cells, these cells are promising devices for photovoltaic applications. In order to optimize their yields, we used the SCAPS-1D program to perform simulations of n- ZnO/p-CuO and n-ZnO/p-Cu_2O thin-film solar cells (Figure 1) by varying certain parameters [1,2,3]. Its parameters which were thickness, bandgap, electron affinity, relative dielectric permitivity, shallow uniform donor density ND, shallow uniform acceptor density NA etc. The short circuit current and efficiency were 28.39 mA.cm^{-2}, 10.44 mA.cm^{-2} and 28.42 %, 16.38 % respectively for cells n- ZnO/p-CuO and n-ZnO/p-Cu_2O (Figure 2). Our results reveal that the n- ZnO/p-CuO solar cell is more efficient than the n-ZnO/p-Cu_2O solar cell and can be used to convert solar energy into electricity.

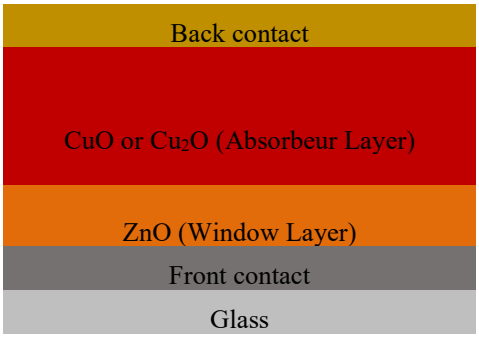

Figure 1. Structure of the solar cell.

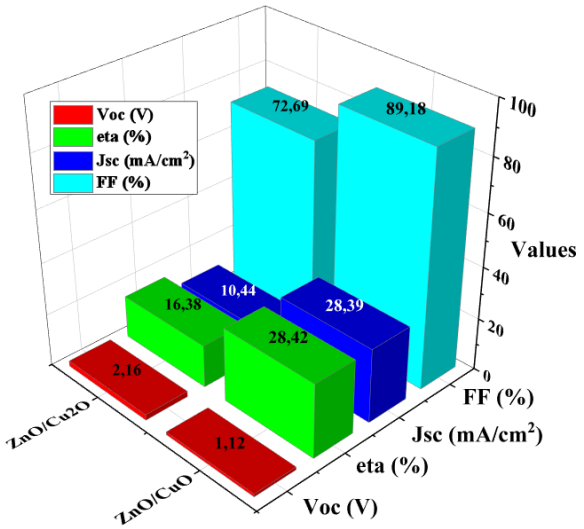

Figure 2. Characteristics parameters of solar cell.

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[3] Sawicka-Chudy P, Sibiński M, Wisz G, Rybak-Wilusz E and Cholewa M, Numerical analysis and optimization of Cu_2O/TiO_2, CuO/TiO_2, heterojunction solar cells using SCAPS, *Journal of Physics* (2018).

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Opportunities and Challenges of Lead-Free Perovskite for high efficiency and stable solar cells with a low-cost technique

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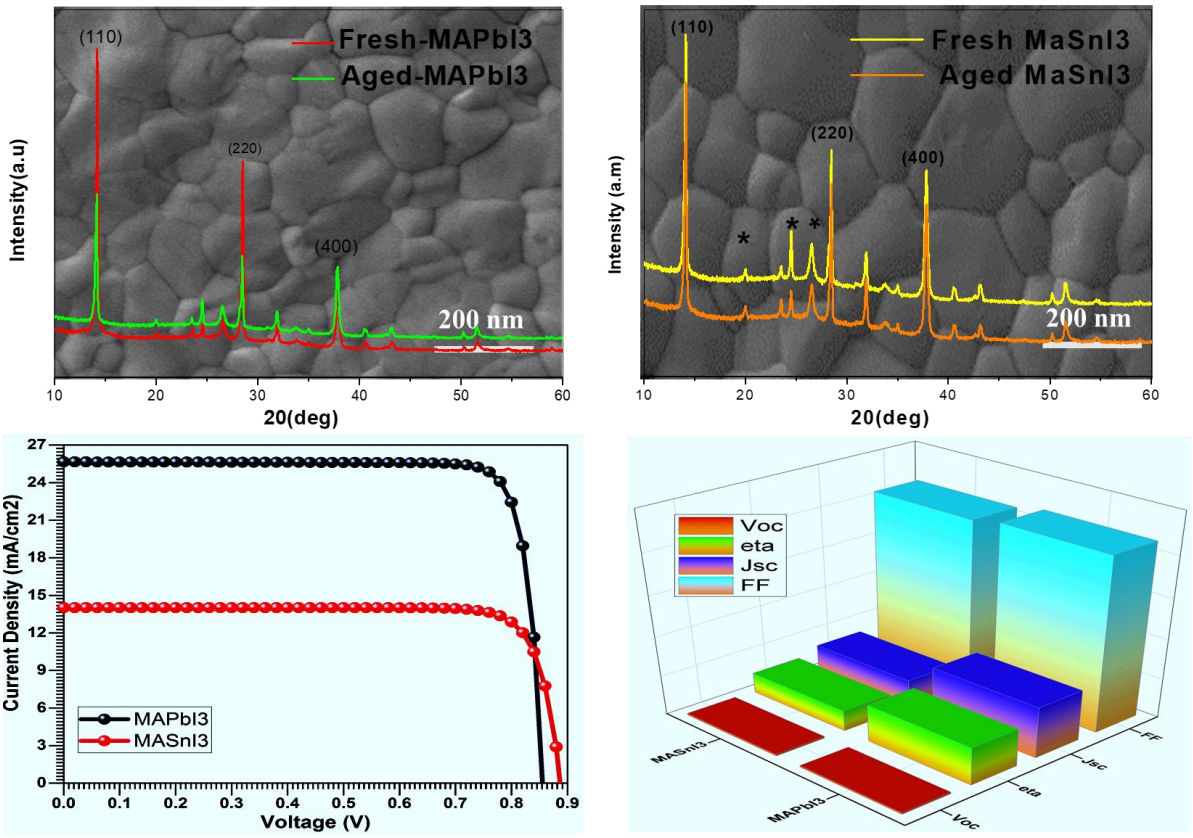
Lead-Free Perovskite is n-type semiconductor material considered a potential candidate with a tunable bandgap used as absorber layer solar cells. The $MASn_{1-x}Pb_xI_3$ samples were successfully prepared by the solution mixed spin coating technique. The XRD analysis revealed the polycrystalline nature of the films. It observed from the morphology that the homogeneity of the films very corresponds to replace Pb with Sn . The AFM analysis showed the big grain and the rough surface of the films. The optical absorption indicates a remarkable shift to the lower wavelength and the optical band gap was found to vary from 1.82 to 1.8 eV with V- doped contents. The measured intensity of the PL peak in $MAPbSn_3$ films is about 30% higher than in $MAPbI_3$ films, We manufacture the Device Manufacture Spiro-OmeTAD/$MASnI_3$/TiO_2/FTO where Voc=0.887 V, Jsc=14.02 mA/cm2, FF=83.72% and eta=10.42%. In perovskite-based devices using MASnI3 as an absorber, it was found to be more stable despite of its lower efficiency, which could be improved by enhancing the bandgap alignment of MaSnI3. The results also allow the development of a new, reliable production system for PSCs

Graphical Abstract



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CIGS solar cell efficiency enhanced by structural engineering at buffer/CIGS interface

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For CIGS-based solar cells with the following structure (ZnO/buffer/p-CIGS/back contact) the most influential interfaces are the (buffer/CIGS) and (CIGS/back contact) interfaces.

In this study we present the results of the numerical simulation of our heterojunction thin film solar cell based on CIGS with two buffer layers less toxic than CdS: $ZnO_{1-x}S_x$ and SnS_2. The SnS_2 in addition to being non-toxic has electrical properties close to CdS such as gap and electronic affinity. $ZnO_{1-x}S_x$ has the advantage of having a variable gap, which allows the discontinuity of the band structure at the buffer/CIGS interface to be modified.

From the optimized Zn(O,S) layer parameters by varying the sulphur content in $ZnO_{1-x}S_x$, we vary the thickness, the carrier concentration of both absorber and buffer layers and propose an structure of our solar cell. The calculations are performed keeping the other parameters constant and considering a p-CIGS/p+-$MoSe_2$/Mo back contact with a work function of the metal Mo = 5.49 eV and a forward reflection R = 5%, using the SCAPS software.

The optimization of the Zn(O,S) buffer layer leads to a sulfur composition S/(O+S) ratio of 0.79 with more enhanced performance for the $Zn(O_{0.30}S_{0.79})$/GIGS contact. Above 0.79 the performance of the solar cell is affected depending on its thickness and carrier concentration. The results after stimulation show that the performance of CIGS-based solar cells with $Zn(O_{0.30}S_{0.79})$ and SnS_2 as the buffer layers are slightly different in terms of efficiency with 23.54% and 23.44% respectively. In addition, there is a difference in the open circuit voltage (Voc) and short current (Jsc) due to the reduction of interface recombination at the $Zn(O_{0.30}S_{0.79})$/CIGS interface and the type of band structure at the buffer/CIGS interface.

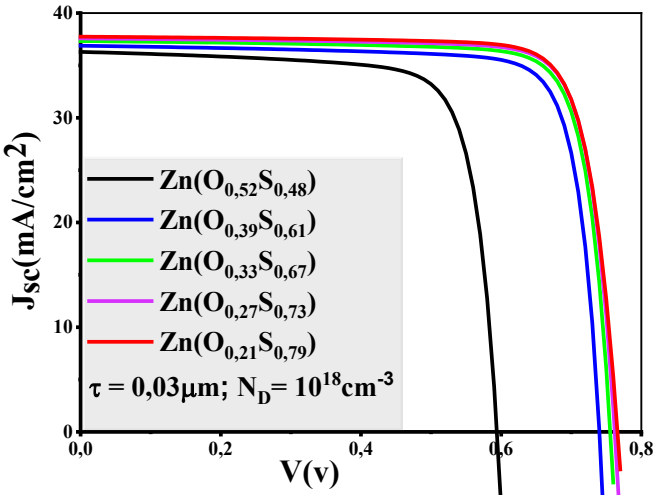

Figure 1. *J -V* curve of S/(S+O) composition ratio.

The compositional and configurational space of spinel nitride solid solutions: accelerated exploration of electronic properties through machine learning

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Solid solutions of spinel nitrides with Group IV cations are very suitable materials for optoelectronic applications, thanks to their outstanding properties like a great hardness and oxidation resistance, plus a wide bandgap range when modifying cations partial concentration. Specifically, tin-germanium nitride solid solutions have been previously reported as promising materials for intermediate band solar cells (IBSC), used as host materials where an intermediate band (IB) could be achieved through transition metal hyperdoping of the optimal host [1]. The finding of an operative material like these could contribute to a groundbreaking change in the field of photovoltaics, because of the ideal efficiency limit of up to 63% that could be obtained with just a single layer configuration.

To be able to efficiently explore the vast compositional and configurational space of these materials to find an optimal host, we have performed a thorough study combining density functional theory (DFT) and machine learning (ML) techniques, aiming at a full and accurate description of the electronic properties for all the possible configurations within the space. The implementation of ML and other statistical analysis techniques allows us to reduce the number of DFT calculations required to fulfill that task, accelerating the process by several orders of magnitude [2]. Mixing energies, to give a broad perspective of thermodynamics and intrinsic stability of the different configurations, as well as accurate bandgaps, obtained through correlation of some HSE results and more basic DFT calculations, are successfully reproduced by the ML models. We test several statistical models with different complexity levels and a variety of atomic-level descriptors based on structural information in the process. Our results demonstrate the usefulness of ML for predictions in the configurational space of alloys and show some hints about most suitable methods and descriptors for different target systems and properties.

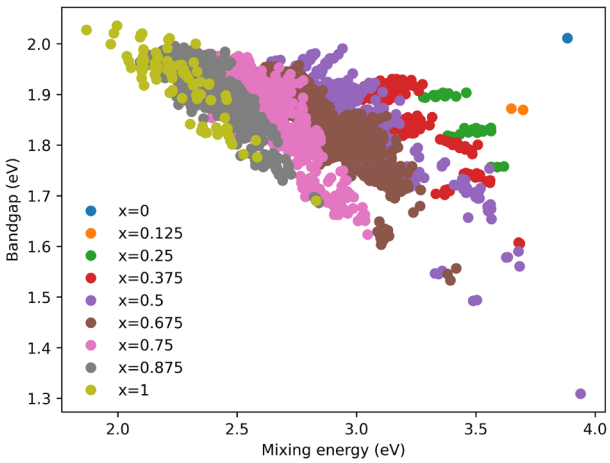

Figure 1. Distribution of predicted mixing energies and bandgaps for all the inequivalent configurations and different inversion.

[1] P.Sánchez-Palencia. G.García, J.C.Conesa, P.Wahnón, P.Palacios, *Acta Materialia* **197**, 316 (2020).
[2] S.D.Midgley, S.Hamad, K.T.Butler, R.Grau-Crespo, *Journal of Physical Chemistry Letters* **12**, 5163 (2021).

Acknowledgements: This work was accomplished thanks to the mobility grants given by Universidad Politécnica de Madrid Programa Propio de I+D+I 2021 and ERASMUS+ european project. P.S-P., as presenting author in this communication, also acknowledges support from Ministerio de Ciencia e Innovación through the project BESTMAT-QC (PID2019-107137RB-C22).

The 2030 power sector transition in Spain: advantages and drawbacks of massive deployment of solar photovoltaic sources

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This work deals with the 2030 power transition in Spain to accomplish with the European Union (EU) target of reaching climate neutrality by 2050. In this line, the EU has realised that if we want to implement the agreements of not increasing the globe temperature in more than 1.5°C, then the program of eliminating carbon emissions or to reach the Net Zero Emissions has to be accelerated.

Within this context, we analyze in this work the plan established by the Spanish government under the umbrella of the National Plan for Energy and Climate (so-called PNIEC) which fixes very clear objectives for our electricity power system. This Plan is originally based in a very large development of renewable energies which in 2030 will boost the amount of solar photovoltaic (PV) and wind adding up to 73 % of the total mix.

Nonetheless, this large deployment of PV, about 3 times the present value, is not free of controversy due to the massive need of storage capacity and/or backup power plants with very flexible and fast ramping response. Making use of historical data, we present in this work a forecast of the 2030 scenario with some suggestions and recommendations.

To evaluate the impact of high deployment of variables renewable sources, and particularly the effect of large increase of solar photovoltaic we make use of the analysis proposed by [1] based on the *duck curves* presented in Figure 1 and 2.

The relevance of future research opportunities is presented in the last section of this article.

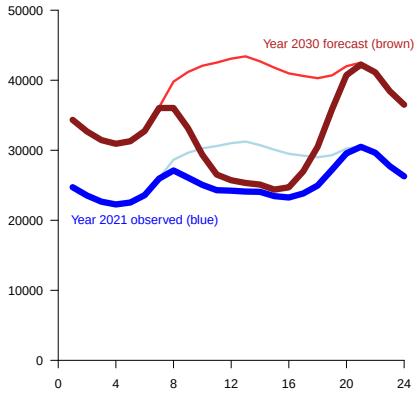

Figure 1. Comparative of present vs 2030 estimated duck curves. Source: Authors

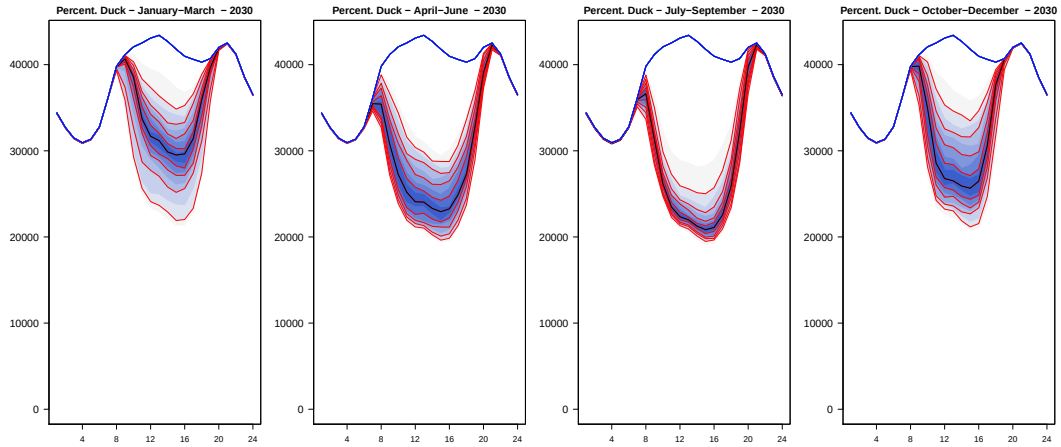

Figure 2. Seasonal percentiles fan-charts of duck curves for the 2030 forecast in Spain. Source: authors.

[1] Denholm, P., O'Connell, M., Brinkman, G., & Jorgenson, J. (2015). Overgeneration from solar energy in California, a field guide to the duck chart. *National Renewable Energy Lab*, Golden, CO (United States).

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