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Simulation of NiO_x Based Solar Cells Using SCAPS Software

Arya Krishnan and T.D. Subash*

Department of Electronics and Communications Engineering, VISAT Engineering College, Ernakulam, Kerala, India

***Correspondence to:**
T.D. Subash
Department of Electronics and Communications Engineering,
VISAT Engineering College,
Ernakulam, Kerala, India.
E-mail: deanresearch@visat.ac.in

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Abstract

In this paper, the SCAPS simulator is used to study an n-i-p NiO_x (Nickel oxide) based solar cell. This paper proposes a NiO_x based solar cell with perovskite, titanium dioxide (TiO_2) and zinc oxide (ZnO) as four layers and its performance has been studied, using a simulation program called SCAPS-1D software (Solar cells capacitance simulator). Solar cells are widely investigated and used for power generation because of their low manufacturing costs and high conversion efficiencies. NiO_x is one of the most promising inorganic hole transport layers for perovskite solar cells (PSCs) due to its low cost, excellent hole mobility, and superior stability, so they are used.TiO_2 is a low cost and nontoxic photocatalyst. In the visible range, ZnO is a highly conductive thin film with exceptional transparency. The ZnO thickness layer and temperature of cells were evaluated in depth based on the device structure and fabrication method. It has been suggested and numerically simulated to use a planar, regular design with devices configured as NiO_x/perovskite/TiO_2/ZnO. Thickness, an essential absorber layer material parameter, has been altered for examining their impact on device performance. Additionally, the impact of changing temperatures on photovoltaic (PV) performance has been investigated. With a maximum power conversion efficiency of 22.11%, an open-circuit voltage V_{OC} of 1.3 V, a short-circuit current density J_{SC} of 19.44 mA/cm^2, and a fill factor (FF) of 85.25%, the most optimized device performed the best and I-V characteristics of the structure observed.

Keywords

Nickel oxides, Perovskite, Titanium dioxide, Photovoltaic, SCAPS-1D

Introduction

In fact, organic-inorganic PSCs have emerged as a very promising candidate for third-generation solar cell technology. These solar cells possess excellent electrical and optical properties, making them a viable option for efficient energy conversion. Additionally, their economic feasibility in terms of fabrication has contributed to their growing popularity. In recent years, there has been remarkable progress in PSC research, leading to significant improvements in power conversion efficiency (PCE). As of 2017, PCEs as high as 23% have been achieved, indicating the immense potential of this technology. Initially, there was considerable interest in mesoscopic structures for PSCs [1, 2]. However, more recently, there has been a shift towards planar structures, specifically n-i-p (negative-intrinsic-positive) or p-i-n (positive-intrinsic-negative) configurations. This shift is primarily attributed to the structural simplicity of planar structures and their low temperature processability. Flexible structures are particularly desirable for PSCs intended for applications such as flexible electronics. Flexible common substrates like polyethylene naphthalate and polyethylene terephthalate are

susceptible to damage at high temperatures, which are typically required for mesoscopic configurations. In this context, planar configurations offer an advantage as they can be processed at lower temperatures, thus enabling the fabrication of flexible PSCs without damaging the substrates. Furthermore, planar configurations also present opportunities for tandem junction cells using perovskites. Tandem junction cells involve stacking multiple solar cell layers to enhance the overall efficiency of the device. By utilizing planar configurations, perovskite-based tandem junction cells can be realized, opening doors for even higher performance and efficiency. Overall, the shift towards planar structures in PSC research offers advantages such as simplified fabrication, low temperature processability, and compatibility with flexible substrates. These advancements are driving the progress and potential of organic-inorganic perovskite solar cells as a leading technology in the field of solar energy conversion [1].

Nanoscience is a multifunctional discipline that covers broad areas such as nanotechnology and nano-chemistry. Nanotechnology aims at preparing nanoparticles with new properties and developing materials and devices based on them. This is one of the current directions of natural sciences in the 21st century. The development of nano-chemistry is associated with the transition from the microscale to the nanoscale level. The study of nanometric particles has led to the discovery of size effects, which can be considered as a new degree of freedom that gives new qualities to chemical compounds and gives rise to previously unknown chemical transformations. The research evolved in such a way that the first efforts were directed at the study of atoms, clusters, nanoparticles of different metals, semiconductors, fullerenes, carbon nanotubes as well as the physicochemical properties of the respective materials. This led to the first studies in the field of nano-chemistry [3].

Furthermore, access to electricity is closely linked to variousessential aspects of human well-being and development. A reliable and uninterrupted power supply is essential for maintaining good health, as it supports healthcare facilities, enables the operation of medical equipment, and ensures the availability of clean water and sanitation. In agriculture, electricity is crucial for irrigation systems, food processing, and refrigeration, thus enhancing agricultural productivity and food security. Indeed, solar energy is one of the most significant and sustainable sources of energy available to us. Unlike finite fossil fuel resources, solar energy is renewable and virtually inexhaustible [4, 5]. The sun continuously emits an enormous amount of energy that can be harnessed and converted into usable electricity through solar cells. Solar cells, also known as PV cells, are devices that directly convert sunlight into electricity using the PV effect.

When sunlight strikes the surface of asolar cell, it excites electrons in the material, generating an electric current. This electricity can then be used to power various applications and contribute to our energy needs [6]. The growth of the PV market over the pastdecade has indeed been substantial. PV devices, which convert sunlight directly into electricity, have become increasingly popular as a renewable energy source due to their environmental benefits and decreasing costs. One notable advancement in PV technology is the use of semiconductor material layers that are only a few micrometers thick, in contrast to traditional crystalline wafers that are several hundred micrometers thick. This innovation has been driven by the development of thin-filmsolar cells, which can be made using various materials such as amorphous silicon, cadmium telluride, and copper indium gallium selenide. These thin-film solar cells offeradvantages such as flexibility, lightweight design, and the ability to be integrated into various applications. The abilityto deposit thin films on thin substrates, such as flexible plastics or metal foils, has opened up new possibilities forconstructing flexible PV modules [2]. Overall, the combination of thin-film technology, flexible PV modules, and high-throughput deposition methods has driven the growth of the PV market by making solar energy more accessible, versatile, and cost-effective. These advancements continue to contribute to the expansion of renewable energy adoption and the transition towards a more sustainable future [3].

In organic PV devices, commonly known as p-i-n PSC, organic compounds such as PEDOT:PSS (HTM; Hole transport material) and PCBM (ETM; Electron transport material) have been widely studied and utilized as interfacial or transport materials [4]. However, these organic materials do have certain limitationsthat can impact the performance of the solar cells, including poor conductivity, low carrier mobility, high chemical instability, and higher processing costs. To address these limitations, researchers have been exploring alternative materials, particularly inorganic compounds, as substitutes for HTMs and ETMs in PSCs. Inorganic materials offeradvantages such as higher conductivity, improved stability, and potentially lower manufacturing costs [7].

The study he described aims to provide a better understanding of the performance of inorganic metal oxide transport layers as interface materials in planar PSCs. In this work, a 1D simulation-based approach is employed to study the behavior of PSCs with allinorganic metal oxide transport layers in a p-i-n configuration [8]. The chosen high bandgap p-type oxide, NiO_x, serves as the HTM to enhance optical transparency for incoming light. Separately instead considered the different ETM ZnO (oxide with higher conductivity) and TiO_2 (most used material for mesoscopic and n-i-p structures) [9]. Open circuit voltage (V_{OC}), short circuit current (J_{SC}), fill factor (FF) and especially PCE are solar performance parameters that are analyzed for the structure with various fault scenarios and failure states interface with different thicknesses. and temperature variation.

Experimentation

Simulation using SCAPS

A simulation software called SCAPS (Solar Cell Capacitance Simulator) with version 3.3.00, which was originally developed for solar cells made of polycrystalline thin-films, CdTe, and CIGS [1], is used in the simulation. Open-circuit voltage (V_{OC}), short circuit current density (J_{SC}), fill factor (FF%), quantum efficiency (QE%), efficiency percentage, heterojunction energy band structure, etc, are some

of the AC and DC electrical metrics that can be recreated on SCAPS [2]. Any of these measures can be estimated and measured in both light and darkness, at different temperatures.

In our paper we are taking each layer as uniform layer, and we are not introducing any defects. Here four layers NiO_x, perovskite, TiO_2, and ZnO are taken, and the solar cell is simulated. The SCAPS program computes energy bands, concentrations, currents, J-V characteristics, AC characteristics (C as function of V and/or f), and spectral response at a specific working point (also with bias light or voltage) [3]. The left and right contact is given, and light is applied from right contact and voltage is given to left contact and right contact is grounded. Interfaces are also added. First the structure is simulated, and J-V characteristics and C-V characteristics are noted. The SCAP software's numerical portion is depicted in figure 1.

The thin-film planar NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell structure that was built andemployed in the SCAPS simulations is shown in figure 2. The analysis is performed on the effects of the thickness of the perovskite layer. The performance of the NiO_x/perovskite/TiO_2/ZnO planar heterojunction thin-film solar cell under various solar concentrations and operating temperatures was also examined. Table 1 lists the parameters for NiO_x, perovskite, TiO_2, and ZnO that were used in the simulations [6].

Results and Discussion

Simulation of NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell

Figure 3 shows simulation of NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell. Interfaces NiO_x/perovskite, perovskite/TiO_2, and TiO_2/ZnO are added. Figure 4 depicts J-V characteristics of NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell.

Observed J_{SC} = 19.44 mA/cm^2 and module efficiency = 15.56%. Figure 5 shows C-V characteristics of NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell.

Figure 1: The numerical section of SCAP software.

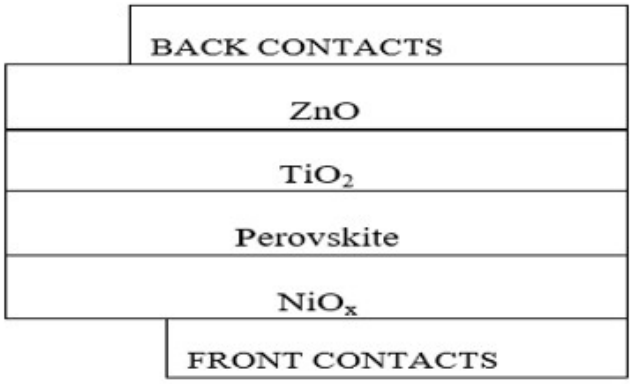

Figure 2: NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell schematic.

Effect of thickness of perovskite layer and temperature variation of solar cell

The thickness of perovskite layer varies from 0.080 micrometer to 1.5 micrometer and the graph is observed. Figure 6 shows batch set up window. In this structure, the short circuit current density reached up to 19.44 mA/cm^2 resulting in 22.11% PCE. Figure 7 and figure 8 show the J-V and C-V

Table 1: Performance of TG-1-BFA-based 4-bit RCA.

Parameter	NiO_2	Perovskite	TiO_2	ZnO
Thickness, d (μm)	0.080	0.320	0.080	0.080
Bandgap, Eg (eV)	3.700	1.600	3.300	3.200
Electron affinity, EA (eV)	2.100	4.100	4.200	4.100
Relative permittivity	10.700	10.000	10.000	8.100
Conductionband effective density of states NC (cm^{-3})	2.000E+19	2.000E+18	2.500E+18	4.500E+18
Valance band effective density of states NV (cm^{-3})	1.000E+19	1.000E+18	1.000E+18	1.000E+18
Electron mobility	1.2000E+1	1.000E+2	1.000E+0	3.000E+2
Hole mobility	2.000E+0	1.000E+1	1.000E+0	1.000E+0
Shallow uniform donor density ND (cm^{-3})	0	1.000E+9	1.000E+19	1.000E+19
Shallow uniform acceptor density NA (cm^{-3})	1.600E+14	1.000E+9	0	0
Electron thermal velocity (cm/S)	1.000E+7	1.000E+7	1.000E+7	1.000E+7
Hole thermal velocity (cm/S)	1.000E+7	1.000E+7	1.000E+7	1.000E+7

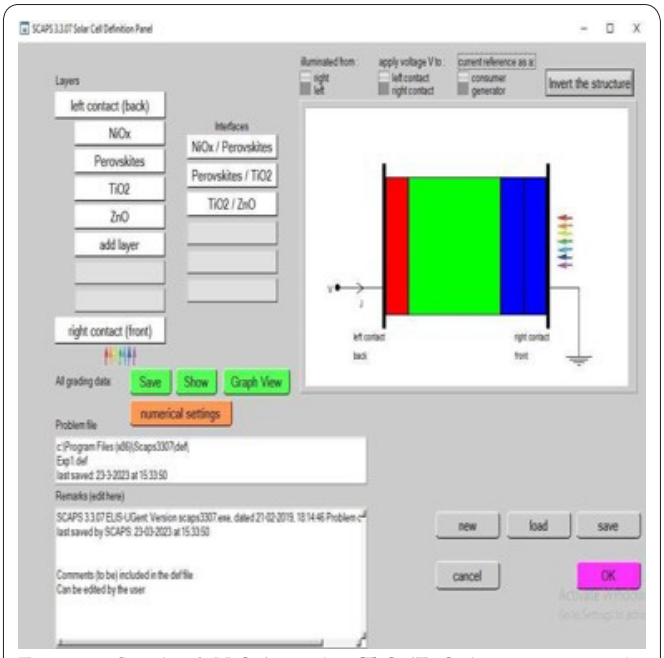

Figure 3: Simulated NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell.

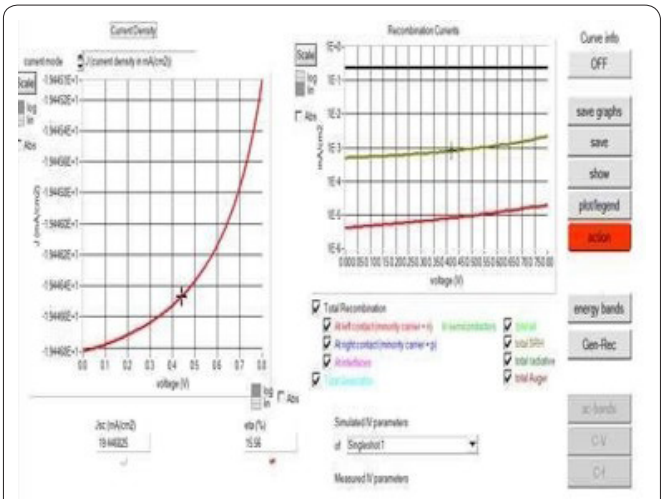

Figure 4: J-V characteristics of NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell.

characteristics of NiO_x/perovskite/TiO_2/ZnO heterojunction cell, respectively.

As varying the operating temperature, the efficiency of the solar cell is observed. The temperature changed from 300 K to 100 K in five steps (400 K, 350 K, 300 K, 250 K, 200 K, 150 K, and 100 K) and J-V characteristics are noted.

From the J-V characteristics it can be observed that by changing thickness and temperature, the efficiency increased from 15.56% to 22.11% where all other parameter values remain unchanged. The structure was found to have almost the same pattern with thickness variation. Since a moreabsorbing layer results in more light absorption, FF increases with thickness. Observed V_{OC} = 1.3334 V, J_{SC} = 19.44 mA/cm^2, FF = 85.25% and module efficiency = 22.11%.

Effect of variation of left contact metal work function

The minimum amount of energy or photons required to

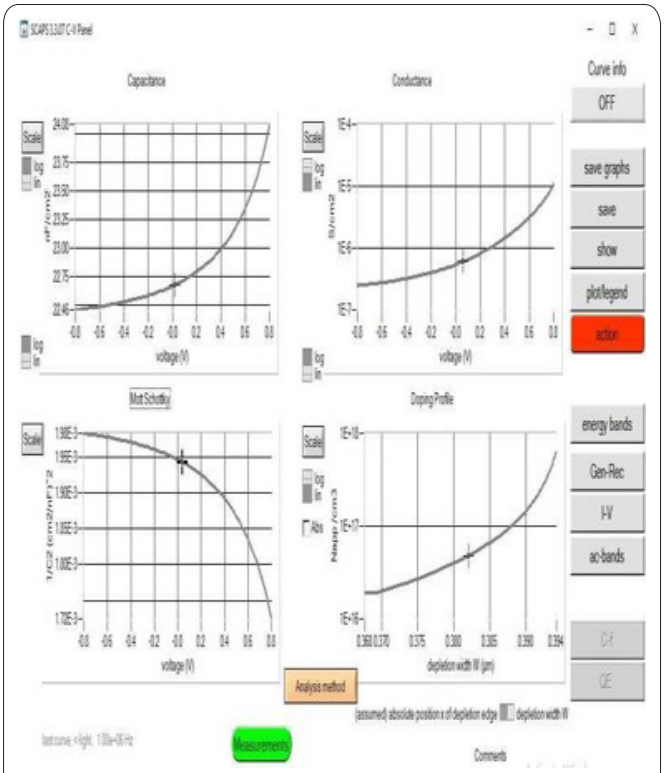

Figure 5: C-V characteristics of NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell.

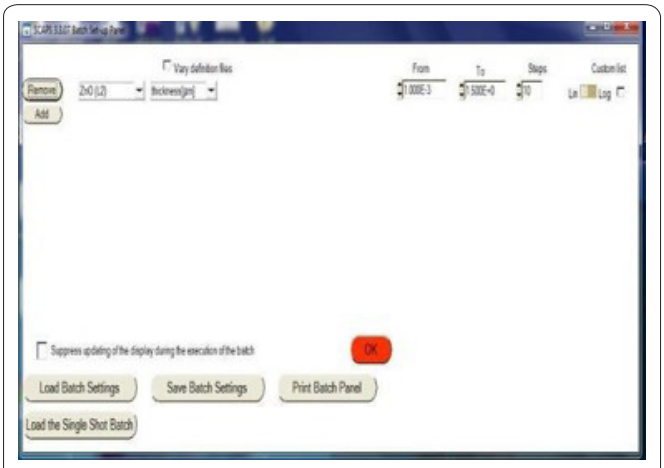

Figure 6: Batch set up window.

ejectan electron from a metal's surface is known as the work function [8]. Figure 9 shows the left contact window and figure 10 shows V_{OC} vs temperature graph.

Here the left contact metal work function is taken as 5 and again calculate the recorder we can observe that the voltage reaches saturation instead of straight line. Without introducing additional defects simulation of the NiO_x/perovskite/TiO_2/ZnO heterojunction solar cells was performed. Variations in the absorber layer's thickness are noted. The perovskite layer's shallow donor density was set at 1.000E+9 cm^3. The TiO_2 layer's shallow donor density was tuned at 1.000E+19 cm^3. The ZnO layer's shallow donor density was tuned at 1.000E+19 cm^3. In the NiO_x layer, the shallow acceptor densities were tuned at 1.600E+14 cm^3 and shallow acceptor densities of perovskite is tuned at 1.000E+9. According to this construction, a short circuit current density of up to 19.44 mA/cm^2 and a power

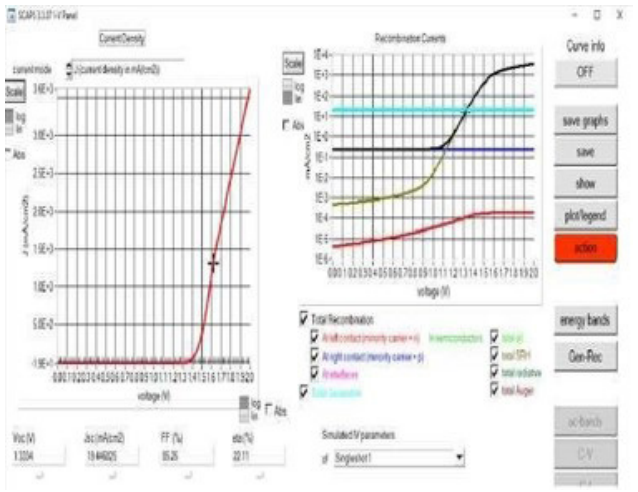

Figure 7: J-V characteristics of NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell using batch setup.

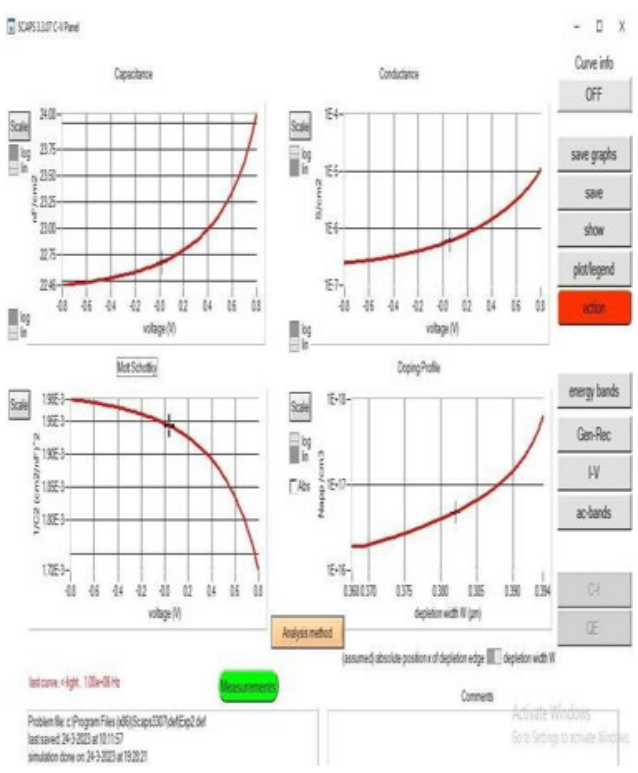

Figure 8: C-V characteristics of NiO_x/perovskite/TiO_2/ZnO heterojunction solar cell.

conversion efficiency of 15.56% can be achieved. By varying thickness of absorber layer and temperature variation increases the efficiency to 22.11%.

Conclusion

The J-V characteristics in various cases of NiO_x/perovskite/TiO_2/ZnO heterojunction structure was observed. ZnO layer thickness is altered, and a graph is drawn. 15.56% efficiency is achieved. It has been found thatthe proposed cell's efficiency can be further increased to 22.11% with the increase in thickness of absorber layer. The effect of temperature and metal work function is also noted, and graph is plotted. The

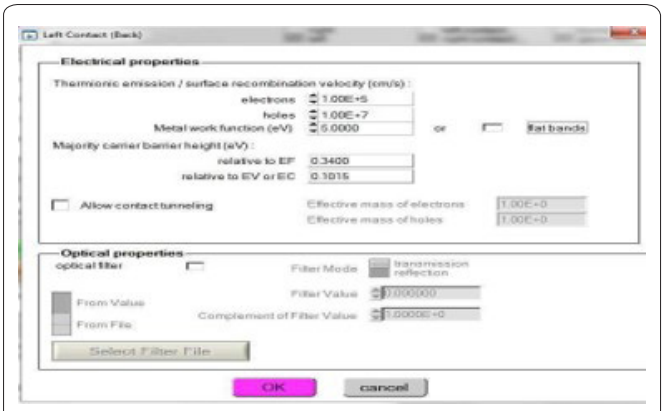

Figure 9: Left contact window.

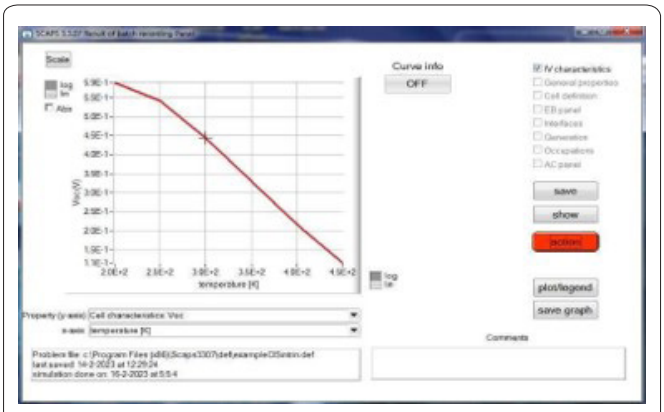

Figure 10: V_{OC} vs Temperature graph.

cell's efficiency again increases to 22.11% and thus we can conclude that an efficient NiO_x based solar cell is obtained.

Acknowledgements

None.

Conflict of Interest

None.

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