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Molarity-Driven Modulation of Li_2O Thin Films for UV-Sensitive Photovoltaic Devices

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Abstract: Li_2O powders were synthesized by the sol–gel method using lithium nitrate solutions of 1.0 M, 0.9 M, and 0.7 M to analyze the effect of precursor concentration on photovoltaic and optical properties. Reflux heating, filtration, and calcination of the samples were followed by analysis through UV–VIS spectroscopy. Optical properties such as absorption coefficient, extinction coefficient, and band gap were determined, and the band gap increased with increasing concentration from 3.410 eV to 3.573 eV. The powders were pasted and coated onto FTO substrates, sensitized by Blue Nile dye, and packaged with graphite-coated counter electrode and iodine electrolyte. I–V measurements under illumination of 0.55 $W \cdot m^{-2}$ showed the 1.0 M sample reached maximum efficiency (0.903%), resulting from the stronger absorption and narrower band gap of the sample. Films with lower concentration had decreased photovoltaic performance. These findings show that Li_2O content significantly impacts optical properties and solar cell efficiency, offering a direct route to improving Li-based material performance in low-light photovoltaics.

Keywords: *Li_2O Thin Films, Sol–Gel Synthesis, Optical Properties, Photovoltaic Efficiency, and Precursor Concentration.*

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I. INTRODUCTION

The rapid consumption of fossil fuels and mounting anxiety about environmental sustainability have increased the search for clean and green energy resources [1]. Solar power is one of them, a very facile and omnipresent source of energy. Photovoltaic devices are a method of direct conversion of solar energy to electricity; however, cost-effectiveness, stability, and efficiency of photovoltaic devices are still under study and development. In the last couple of years, the use of metal oxide semiconductors in solar cells has drawn phenomenal attention due to their unique optoelectronic properties, thermal and chemical stability, and compatibility with low-cost synthesis techniques [2,3].

Lithium metal oxides, particularly lithium oxide (Li_2O), are gaining interest in optoelectronic and solar photovoltaic devices [4]. Li_2O is a semiconductor with superb visible transparency and tremendous UV absorbance. It is thus a good potential candidate for application in transparent conductive layers, window layers, or even light-harvesting components of UV-sensitive solar cells [5-7]. Additionally, its non-toxicity, earth abundance, and chemical stability further make Li_2O a green and eco-friendly material choice [8].

While there has been promising research on lithium-containing or -comprising oxides such as Li_2TiO_3 and $LiZnO_3$ for applications in photovoltaic devices, that for pure Li_2O as an active layer in solar cells is relatively scarce [9]. Most of the studies to date have been mainly for Li_2O in

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multilayer or doped applications, where it can be utilized mainly as a buffer or as an interface material [10-12].

This research closes this gap by examining Li_2O thin films in isolation, which were prepared at different precursor concentrations (1.0 M, 0.9 M, and 0.7 M). A controlled, sol-gel-derived synthesis method was employed to make films of different optical thickness and morphology. Optical properties, i.e., optical absorbance, transmission, absorption coefficient (α), extinction coefficient (k), and optical band gap (Eg), were also explored in the UV-visible region. Moreover, photovoltaic efficiency of each film was also tested by current–voltage (I–V) analysis under controlled low-level illumination (0.55 $W \cdot m^{-2}$), imitating real diffuse light conditions. Through the identification of a correlation between precursor concentration, optical properties, and solar cell efficiency, this work provides real-world insight into the manner in which small variations in the synthesis conditions can be utilized to manipulate the optoelectronic properties of Li_2O thin films. The work contributes to the list of publications on lithium-based oxides and their potential for exploitation in future low-cost photovoltaic devices.

II. METHOD

Li_2O powder samples were synthesized using sol- gel technique Li_2O powder samples were synthesized by dissolving lithium nitrate ($LiNO_3$) in acidic deionized water to create three precursor solutions with corresponding concentrations of 1.0 M, 0.9 M, and 0.7 M. The solutions were stirred at room temperature for 30 minutes and then refluxed under heat in a water bath for 90 minutes The precipitates thus formed were filtered employing a vacuum pump and calcined at 600 °C for 2 hours. The dried solids were ground into extremely fine powders and calcined once more at 400 °C for 6 hours to obtain the final Li_2O samples.

The optical properties of the powders synthesized were studied using a UV–VIS spectrophotometer between 200 and 800 nm and absorbance, transmittance, and band gap energies were calculated. The powder samples were then mixed with acetone and ground to form a paste, which was applied manually on pre-cleaning FTO glass substrates using a glass rod. The substrates were coated and baked at 100 °C for one hour, then sensitized with Blue Nile dye. Counter electrodes were prepared by coating graphite on the conductive face of FTO glass. The solar cells were assembled by sandwiching graphite-coated FTO glass and dye-coated film with iodine electrolyte between them, also secured with binder clips.

The fabricated cells were exposed to a light intensity of 0.55 $W \cdot m^{-2}$. The current–voltage (I–V) measurements were recorded with the assistance of an external circuit containing (voltmeter, Ammeter, a light source "Lamp", and a solar cell), and key photovoltaic parameters such as Isc, Voc, FF, and η were calculated to analyze the performance of different samples of Li_2O.

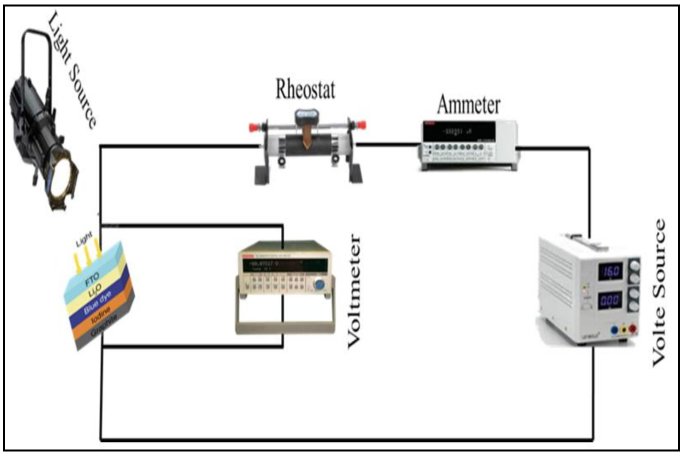

Fig 1 Schematic Diagram of IV Circuit of Thin Film Solar Cell.

III. RESULTS & DISCUSSION

This study investigates how varying precursor concentrations (1.0 M, 0.9 M, and 0.7 M) affect the band structure of Li_2O samples by examining their optical properties.

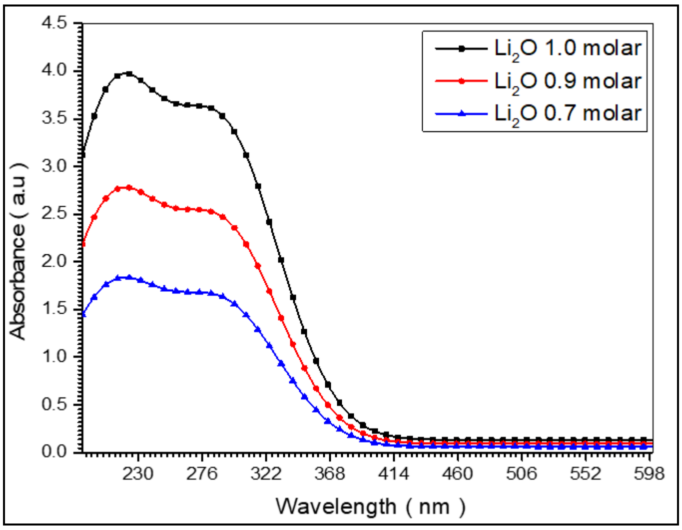

Fig 2 The Abosorbance of LiO_2 Thin Films

Li_2O thin films exhibit clear precursor concentration dependence in the absorption spectra, demonstrating the effect of material loading on optical behavior. All the samples, synthesized from concentrations of 1.0 M, 0.9 M, and 0.7 M, have intense UV absorption, and absorbance becomes lower with higher wavelengths approaching the visible region. This is characteristic for wide-band-gap semiconductors, for which higher energy photons are readily absorbed.

From fig. (2), among the three, the highest absorbance across the UV-visible region is exhibited by the sample prepared with 1.0 M precursor concentration, followed by those prepared with 0.9 M and 0.7 M, respectively. This is because of higher thickness or higher density at higher precursor concentrations, which leads to higher photon absorption owing to higher volume of the absorbing material.

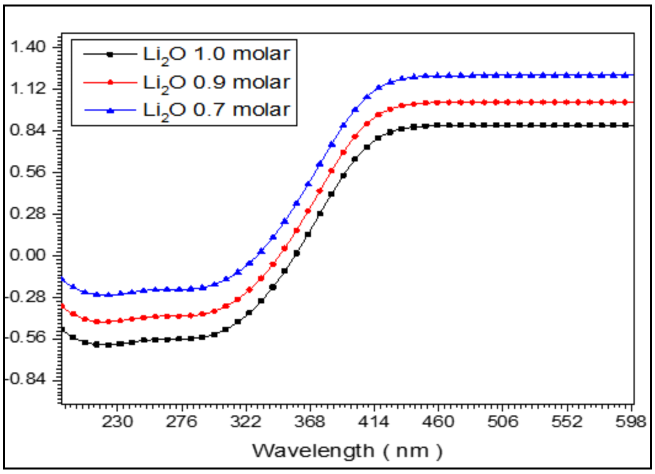

Fig 3 The Transmission of Lio_2 Thin Films

The optical transmission spectra of Li_2O thin films also exhibit concentration-dependent optical behavior observed previously in the absorbance data. Fig. (3) showed that the optical transmittance is enhanced across the UV-visible region with decreasing precursor concentration. This is as would be expected, as thinner or less dense films absorb and scatter light to a lesser extent, and so more photons are capable of transmitting. Among the three samples, the samples produced from 0.7 M concentration exhibited the highest transmittance, particularly in the visible region. This corresponds to a relatively low optical density, as is agreed by its lower absorbance and broader optical band gap. On the other hand, the 1.0 M sample exhibited the lowest transmittance, which is agreeable with a thicker or denser film that would absorb more of the incident light. From a photovoltaic standpoint, reduced transmission in the more concentrated films is desirable. It is a sign of more concentrated light absorption, as required for ideal photocurrent generation. In contrast, the higher transmission of the 0.7 M sample, while a sign of greater optical clarity, is a sign of reduced light-harvesting capability and hence lower photovoltaic efficiency.

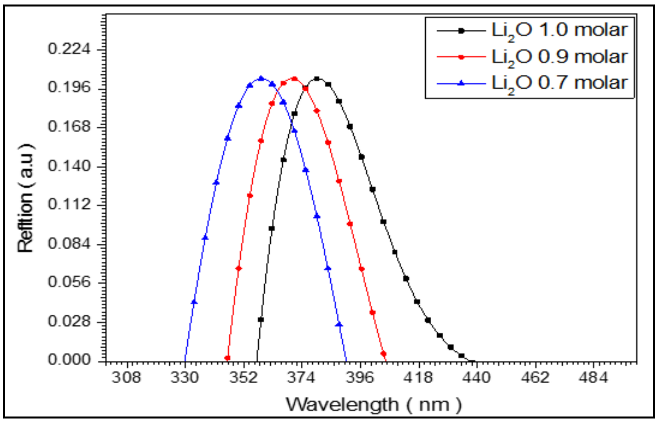

Fig 4 The Reflection of Lio_2 Thin Films

Reflectance spectra of Li_2O thin films contain further information regarding the effect of film composition on their light-incident interaction. Fig. (4) demonstrate that similar to the absorbance and transmission results, reflectance is dependent on precursor concentration. In most cases, all samples have relatively low reflectance over the UV-visible spectral range, which is favorable for photovoltaic devices in the sense that less light is reflected and more can be absorbed or transmitted. Among the samples, the sample made from the highest concentration (1.0 M) has a slightly higher reflectance than the 0.9 M and the 0.7 M samples. This may be due to higher film thickness or surface roughness, which may lead to greater scattering and reflection at the surface. The reflectance values are nevertheless very small, reflecting good optical coupling of light into the films. Conversely, the 0.7 M sample is the most reflective, and this may be due to its smoother, thinner nature or lower density. While low reflectance is always a good thing in terms of increasing light trapping in solar cells, in this case, it is accompanied by reduced absorbance, so additional light passes out of the film without being absorbed. This trend focuses on the necessity of compromising less reflection with sufficient film thickness and density so as to achieve efficient absorption. In this context, 1.0 M film appears to achieve the optimal compromise by keeping reflectance low while optimizing absorbance, which is evident in its enhanced photovoltaic performance.

The absorption coefficient (α) of Li_2O thin films was probed in order to understand their optical properties more deeply and to study the effect of precursor concentration on light–matter interactions. The coefficient was determined from absorbance by the formula:

$$\alpha = \frac{2.303 \times A}{t}$$

where (A) is the absorbance and (t) is the optical length in the samples [13].

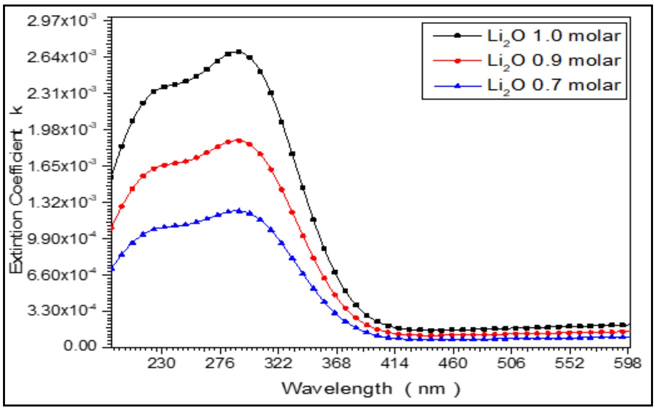

Fig 5 The Absorption Coefficient of Li_2O Thin Films

Across the UV-visible spectrum, all Li_2O films revealed high absorption coefficients in the ultraviolet, their values decreasing steadily as the wavelength moved towards the visible region. As shown in fig. (5), the sample prepared with 1.0 M concentration always registered the highest α values, which represent increased photon absorption—most likely because of increased material density and thickness. The 0.7 M film, conversely, registered the lowest α values, due to its less dense, thinner profile. In the short wavelength high-energy UV region, absorption coefficients ranged from 10^4 to $10^5 cm^{-1}$as anticipated to support Li_2O's high

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absorption characteristic in the same range. These kinds of high values play a significant role in driving electronic transitions that fuel the production of photocurrent in solar cells.

The extinction coefficient (k) is closely associated with the absorption coefficient (α) and can be calculated by using relationship [14]:

$$k = \frac{\alpha\lambda}{4\pi}$$

Extinction coefficient is a quantitative measure of how the intensity of light diminishes with the velocity of material it is traveling through. The bigger k is, the bigger is light reduction, typically caused by more absorption or internal scattering. Fig. (6) Extinction Coefficient (k) of Li_2O thin films

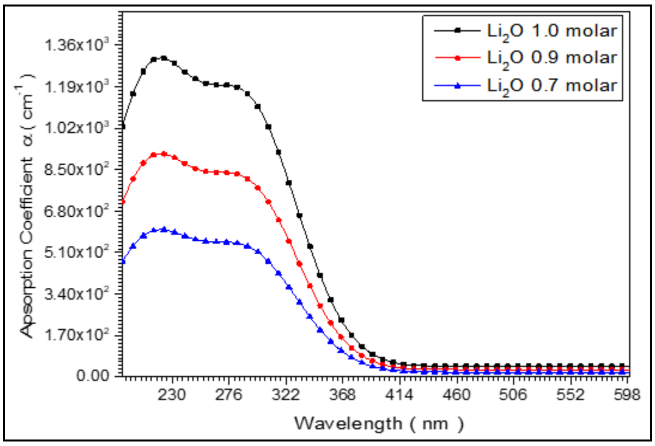

Fig 6 Extinction Coefficient (k) of Li_2O Thin Films

For Li_2O samples, extinction coefficient was seen to reduce with higher wavelength, i.e., the materials get optically most active in UV. For all samples, maximum values of extinction coefficient occur in 1.0 M sample, particularly in UV. This is consistent with its higher absorbance energies and absorption coefficient, i.e., denser or thicker film structure with higher capability for light absorption. Fig. (6) illustrates that with decrease in precursor concentration from 1.0 M to 0.7 M, extinction coefficient values decrease considerably. That is, lesser concentration, thinner films allow lighter to pass through them since the material density and film thickness are smaller. Such properties are also corroborated by patterns of the absorption and transmission spectra. The concentration plays a significant role in driving electronic transitions that fuel the production of photocurrent in solar cells.

The optical band gap (Eg) of Li_2O thin films was determined from the Tauc's plot method based on analysis of the absorption coefficient-photon energy for direct allowed transitions. Utilizing a plot of $(\alpha h\nu)^2$ vs hν, and extrapolation of the linear region of the curve to the energy axis, the band gap values were obtained for films grown at different precursor concentrations [13].

From fig. (7), The band gaps calculated were 3.410 eV for the 1.0 M sample, 3.496 eV for the 0.9 M sample, and 3.573 eV for the 0.7 M sample. The trend of band gap increase with decreasing concentration is indicative of a blue shift to shorter wavelengths in the absorption edge, well referred to as a blue shift. This is due to quantum confinement effects, particularly in the case of thinner or less concentrated films, where decreasing grain size can cause the band gap to become more massive. Additionally, crystallinity, film thickness, and chemical composition alteration at lower concentrations can be the cause of such an effect through a modification of the electronic structure of the material. These findings suggest the tunability mechanism of the optical band gap of Li_2O films by controlling the concentration, where the deeper band gap of the 1.0 M sample is advantageous especially in solar cell applications due to its capacity for absorbing more of the solar spectrum.

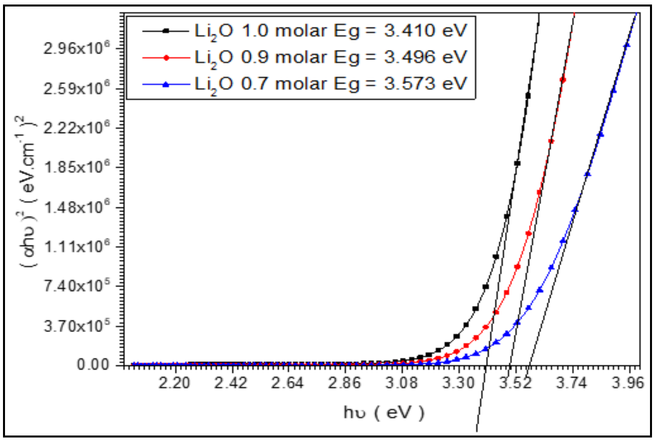

Fig 7 Optical Band Gap (Eg) of Li_2O Thin Films

The I–V characteristics of Li_2O-based solar cells prepared were measured under illuminations of 0.55 $W{\cdot}m^{-2}$. The Photovoltaic characteristics of I–V curves measured are short-circuit current (Isc), open-circuit voltage (Voc), voltage and current at maximum power point (Vm, Im), fill factor (FF), power conversion efficiency (η), and short-circuit current density (Jsc). The result indicates that the device performance is highly correlated with Li_2O concentration. From fig. (8), among the three samples, 1.0 M Li_2O sample exhibited the highest power conversion efficiency of 0.903% with Isc of 5.991 mA, Voc of 0.582 V, Vm of 0.545 V, and FF of 0.89. Nevertheless, the 0.9 M and 0.7 M samples also showed efficiencies of 0.867% and 0.835%, respectively, with comparatively lower Isc and FF values. The Voc was almost constant (~0.582–0.584 V) for all samples, demonstrating intrinsic potential and junction quality for all the concentrations. The same pattern of efficiency is observed in the case of the optical absorption feature mentioned earlier as well. The 1.0 M film with maximum and minimum band gap optical exhibited the highest number of carriers generated under illumination, which translated into higher photocurrent and efficiency overall. The 0.7 M film with the larger band gap and lower absorbance had fewer carriers and therefore lower efficiency.

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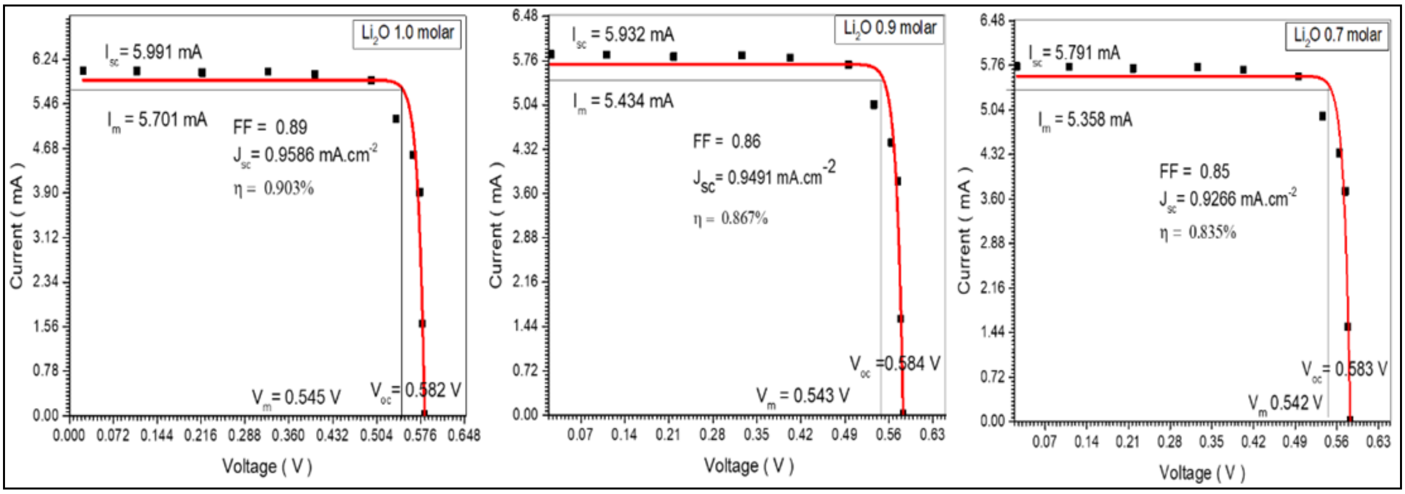

Fig (8) Current–Voltage (I–V) Characteristics of Li_2O-Based Solar Cells at Different Concentrations (1.0 M, 0.9 M, 0.7 M)

Table 1 Photovoltaic Parameters of Li_2O Solar Cells at Varying Precursor Concentrations Under 0.55 w·m⁻² Illumination.

Cell Parmeter	Samples		
	Li_2O 1.0 molar	Li_2O 0.9 molar	Li_2O 0.7 molar
I_{sc}(mA)	5.991	5.932	5.791
I_m (mA)	5.701	5.434	5.358
V_m (V)	0.545	0.543	0.542
V_{oc} (V)	0.582	0.583	0.584
FF	0.89	0.86	0.85
J_{sc} (mA.cm^{-2})	0.9586	0.9491	0.9266
Eg (eV)	3.410	3.496	3.573
η%	0.903	0.867	0.835

Although the reported efficiencies here are relatively low, it must be remembered that they are normalized to the 0.55 $W \cdot m^{-2}$ reduced incident power density. The prospects of the 1.0 M Li_2O device are more apparent when scaled proportionally to normal illumination conditions. These results highlight the observation that increased concentrations of Li2O improve the optical and electrical qualities of the films, rendering them more suitable for photovoltaic devices.

IV. CONCLUSION

This research successfully demonstrated the significant impact of precursor concentration on the photovoltaic and optical properties of sol–gel Li_2O fabricated thin films. The optical and photovoltaic properties were optimized to achieve a denser thicker film having high absorbance in UV, with enhanced extinction and absorption coefficients, and reduced optical band gap by varying lithium nitrate precursor concentration from 0.7 M to 1.0 M. These optimizations were then directly translated to better photovoltaic performance, and the best power conversion efficiency of the 1.0 M Li_2O-based solar cell under low illumination (0.55 $W \cdot m^{-2}$) was found to be 0.903%. Low overall efficiencies aside, trends suggest precursor concentration optimization to be a realistic and simple method to optimize Li_2O film optoelectronic properties for application in solar cells. The findings illustrate the potential of Li_2O as an inexpensive, earth-abundant material for low-light photovoltaics and leave room for enhancement of optimizing the device to its fullest extent under practical light illumination conditions.

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