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Harnessing inorganic silica frameworks: hydrothermal synthesis of POSS nanocages for enhanced efficiency in silicon solar cells

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ABSTRACT

As global population growth and rising energy demands coincide with fossil fuel depletion and escalating environmental degradation, renewable energy sources, particularly solar energy, have become critically important. Silicon solar cells, expected to dominate the market for the next two decades, represent a primary solution. In contrast to conventional approaches focused on modifying the internal structure of silicon solar cells, this study employed a surface modification strategy using a hybrid inorganic, organic nanocoating, based on polyhedral oligomeric silsesquioxane (POSS), a nanocomposite featuring a silica (SiO_2)-like inorganic cage core functionalized with organic amine groups. The silica-based POSS nanocomposite was synthesized via hydrothermal processing and characterized using Fourier Transform Infrared Spectroscopy (FT-IR). Ultraviolet–visible spectroscopy (UV-VIS) spectroscopy confirmed the coating's high optical transparency. Adhesion to the silicon substrate, assessed via pull-off testing, was moderate. Crucially, performance evaluation using a solar simulator demonstrated a 9.32% enhancement in solar cell efficiency following application of the silica-derived coating. This inorganic-enhanced surface modification presents a viable route for improving existing solar cell technology and contributing to global pollution reduction efforts.

Keywords: *Coating, Organometallic compounds, POSS, Renewable energies, Solar cells..*

1. Introduction

The growing global population and escalating energy demands have intensified the need for sustainable and environmentally responsible energy sources. Compounding this urgency are the diminishing reserves of fossil fuels and the grave environmental consequences of their use, particularly the accelerating accumulation of greenhouse gases (GHGs) such as carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O). These emissions contribute significantly to global warming and destabilize the Earth's climate system, leading to profound socio-economic consequences, including reduced agricultural productivity, increased public health risks, and damage to critical infrastructure such as energy grids, transportation networks, and water systems. In response to the intensifying frequency and severity of climate-related disasters, such as extreme heatwaves, floods, droughts, and wildfires, there is a pressing imperative to transition toward clean, renewable energy technologies and achieve deep decarbonization across sectors, in alignment with the targets set by the Paris Agreement and recent Intergovernmental Panel on Climate Change reports. In this context, policymakers, scientists, and industry leaders have increasingly focused on transformative technologies such as carbon capture, renewable energy systems, and circular economy models to redesign the energy landscape [1-4]. Among renewable energy technologies, solar energy has emerged as the most widely utilized and critical resource in the transition toward sustainable energy production. Among these, solar energy has emerged as the most accessible and rapidly scalable renewable source, playing a pivotal role in global sustainability efforts (Figure 1). In particular, solar photovoltaic (PV) technologies have witnessed significant advancements, driven by enhanced conversion efficiencies, reduced production costs, and favorable government incentives aimed at reducing fossil fuel dependency [5].

A key objective in the development of solar technology is the design and deployment of high-efficiency solar cells, as efficiency directly influences both technical performance and economic viability. Higher conversion efficiencies translate into more effective use of installation space, reduced levelized cost of electricity (LCOE), and improved investment returns across various system scales [6-11]. However, efficiency is not the only important factor to consider when designing and selecting solar cell technologies. Economic factors, including production, installation, and maintenance costs, significantly influence market expansion. Additionally, the operational lifespan of solar technologies is a critical determinant of their sustainability and suitability for large-scale, long-term energy infrastructure projects [6-11]. Currently, the photovoltaic industry is dominated by silicon wafer-based solar cells, available primarily as monocrystalline (mono-Si) and polycrystalline (poly-Si) forms. Their physical robustness, long-term stability, and high efficiency have made them the cornerstone of the global solar market. In addition to crystalline silicon, several other solar cell technologies have been developed, including amorphous silicon, cadmium telluride, gallium arsenide, organic photovoltaics, dye-sensitized solar cells, and perovskite-based devices.

Silicon-based solar cells are especially valued for their high efficiencies, typically ranging from 18% to 24%, and long operational lifetimes exceeding 25 years. They also offer relatively low annual degradation rates and are amenable to cost-effective, large-scale production. Owing to these advantages, more than 90% of the global PV market currently relies on crystalline silicon technologies [12-14]. Despite its many advantages in reducing reliance on fossil fuels, the

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large area required for installing photovoltaic panels remains a major obstacle to the widespread adoption of solar energy. Nevertheless, the widespread deployment of solar panels introduces land-use challenges, particularly due to the large surface area required for installations. This has led to growing concern over the competition between land allocated for energy production and agricultural use, particularly in densely populated or land-scarce regions [14-17]. This tension has sparked discourse around the "energy-food land-use conflict," which posits that without adequate planning and technological integration, such as agrovoltaic systems that combine agriculture and solar power, renewable energy expansion could inadvertently compromise food security. To address this, researchers have concentrated not only on enhancing the efficiency of silicon-based solar cells but also on addressing broader systemic challenges by developing innovative materials and advanced design strategies [14-17]. Beyond material selection, geometrical and structural modifications in solar cells have also shown promise in enhancing performance. Conventional silicon solar cells reflect nearly 30% of incident sunlight, a loss that significantly limits energy conversion. Since light reflection varies with photon wavelength, considerable research has been dedicated over the past two decades to improving light trapping, broadening spectral response, and minimizing reflection through engineered surfaces.

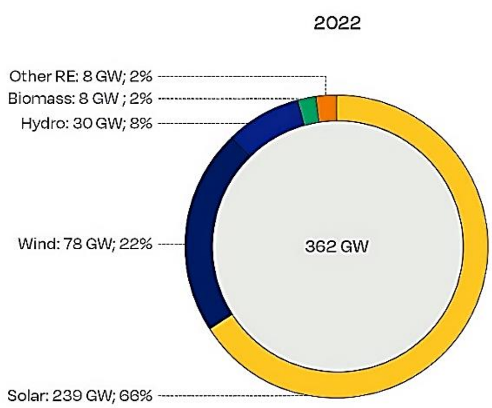

Figure 1. Net capacity of renewable electricity generation until 2022 [5].

Anti-reflective coatings (ARCs), enhanced by nanotechnology, have emerged as key components in this effort. Various nano- and micro-structured designs, such as nanocones, nanogratings, pyramids, nanopillars, nanodomes, nanotubes, and microlens arrays, have been explored to optimize light absorption. However, the application of these coatings is often constrained by processing complexities and scalability issues. While alternative, simpler coating methods have been developed, the incremental efficiency gains often remain modest, and cost considerations must be factored into their adoption In the pursuit of optimal solar cell design, a balance among efficiency, durability, cost-effectiveness, and structural versatility is essential. This interdisciplinary challenge requires insights from materials science, nanotechnology, photonics, and electrical engineering. One class of nanomaterials that has recently garnered attention in this context is polyhedral oligomeric silsesquioxanes (POSS). POSS molecules feature a distinctive three-dimensional cage-like architecture consisting of a silica (Si-O-Si) core surrounded by organically functionalized peripheral groups. This hybrid structure combines the thermal and mechanical stability of inorganic silica with the chemical versatility of organic moieties. Due to their nanoscale size (typically ranging from ~0.5 to 3 nm), high mechanical strength, and tunable optical and electronic properties, POSS compounds are promising candidates for incorporation into various layers of solar cells, including active, interfacial, or encapsulation layers.

Building on these structural and functional advantages, researchers have demonstrated that incorporating POSS into solar cell architectures can enhance light absorption and reduce surface reflection, thereby improving overall energy conversion efficiency. As hybrid organic–inorganic nanostructures, POSS exhibit a unique combination of properties, including thermal stability, mechanical robustness, and surface functionalizability, that make them suitable for diverse applications such as coatings, elastomers, thermoplastics, and thermosets. In the realm of modern nanotechnology, POSS chemistry has emerged as a rapidly evolving discipline. The synthesis and integration of these nanoscale architectures represent a paradigm shift in materials science, offering transformative potential across multiple industries, including construction, aerospace, biomedicine, pharmaceuticals, agriculture, and transportation [18].

At the molecular level, a typical POSS unit comprises a cubic silsesquioxane cage consisting of eight silicon atoms positioned at the vertices, each bonded to three oxygen atoms and a functional organic substituent. This modular architecture enables a wide range of organic modifications, facilitating the synthesis of a diverse library of POSS derivatives with tailored physicochemical properties (Figure 2) [18]. In the context of solar energy technologies, such versatility offers a promising pathway to integrate the advantageous features of both organic and inorganic materials, thereby bridging the performance and stability gap between conventional photovoltaic systems.

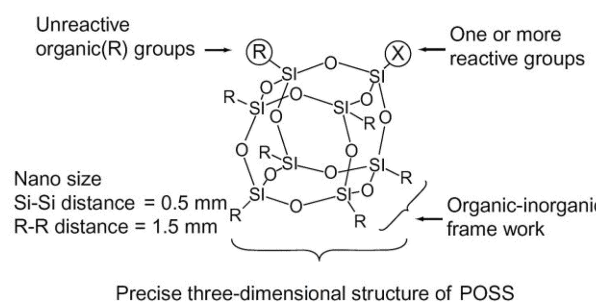

Figure 2. Schematic structure of POSS [18].

The aim of the present work was to enhance the performance of polycrystalline silicon solar cells through surface modification using a transparent amine-functionalized POSS nanocoating. The nanocomposite was synthesized via hydrothermal processing and characterized using Fourier Transform Infrared Spectroscopy (FT-IR) and UV-Visible spectroscopy to evaluate its structural and optical properties. Adhesion to the silicon substrate was assessed through pull-off testing, and photovoltaic performance was examined using a solar simulator. The results demonstrated improved light absorption and energy conversion efficiency, confirming the potential of POSS-based coatings as effective surface modifiers in photovoltaic applications.

2. Experimental

2.1. Materials and method

The synthesis of tetraaminopropyl tetramethyl polyhedral oligomeric silsesquioxane (TAPTM POSS) began by combining 0.05 moles of triaminopropyltriethoxysilane (Merck) and 0.05 moles of methyltriethoxysilane (Merck), followed by stirring at room temperature for 10 minutes. Subsequently, 50 mL of tetrahydrofuran (THF) was added, and stirring continued for 30 minutes. Next, 5 mL of aqueous ammonia (28-30%) was introduced. The resulting mixture was transferred to an autoclave and heated at 150 °C for 17 hours. After cooling to ambient temperature (requiring ~17 hours), the solution was transferred to a sample vial. FT-IR analysis (Figure 3) confirmed the presence of crystalline TAPTM POSS in the clear solution.

2.2. Production of GPTMS/TEOS resin

The resin was fabricated using previously reported method [18]. Initially, 40 mL of pure ethanol was used as the solvent. Subsequently, 24.6 g of tetraethyl orthosilicate (TEOS) was added, followed by the gradual addition of 16.8 g of glycidoxypropyltrimethoxysilane (GPTMS) under continuous stirring at room temperature. The mixture was then supplemented with 1.8 g of deionized water and 2.4 g of hydrochloric acid (HCl). The resulting solution was refluxed at 85 °C for 3 hours. After refluxing, a relatively viscous resin was obtained and transferred to the sample storage container for further use.

2.3. Providing coverage

Coating preparation: The prepared resin was combined with an additive at 10 wt% and the resulting mixture was refluxed for four hours. Subsequently, a thin sol-gel coating was applied onto polycrystalline silicon wafers.

2.4. Identification of compounds and analyses

The composition of TAPTM POSS was analyzed using Fourier-transform infrared (FT-IR) spectroscopy. The optical properties of the coating were evaluated by UV-Vis spectroscopy, while its adhesion strength to the silicon solar cell surface was assessed using a pull-off adhesion tester. Additionally, the performance of the solar cells was measured before and after coating application using a solar simulator equipped with a current-voltage (I-V) measurement system to determine the coating's impact on cell efficiency.

2.5. Characterizations

The fabricated material was characterized by FTIR spectroscopy using a Bruker VERTEX 80 (Bruker Optics, Ettlingen, Germany) and by UV-Vis spectroscopy using an Agilent Cary 60 (Agilent Technologies, Santa Clara, CA, USA). These instruments provided detailed insights into the material's chemical structure and optical properties.

3. Results and discussion

The compound TAPTM POSS's Fourier transform infrared spectrum is displayed. Two strong stretching bands are seen in the range 1043 cm^{-1} to 1119 cm^{-1}, which are associated with the $Si-O_{3/2}$ group's absorption and the Si-O-Si group's asymmetric stretching vibration, respectively. Additionally, the symmetric stretching vibrations of the $(R-Si-O_{3/2})_n$ group are correlated with the presence of a medium band in the 470 cm^{-1} region. The $Si-CH_3$ group is present in the region of 1269 cm^{-1}, as indicated by the sharp and elongated peak. Two peaks can be found in the 1409 cm^{-1} and 1444 cm^{-1}, which represent the methyl groups' symmetric and asymmetric bending vibrations, respectively. The presence of medium stretching bands in the regions 2861cm^{-1} and 2928 cm^{-1} is indicative of the aliphatic C-H group's symmetric and asymmetric stretching vibrations. $N-H_2$ group bending vibrations are represented by the peak in the 1578 cm^{-1}, while symmetric stretching vibrations are represented by the absorption band in the 3364 cm^{-1}. Additionally, the bending vibrations of the $N-H_2$ group that occur outside the normal plane are linked to the absorption peak found at 773 cm^{-1}. C-N stretching vibrations are the cause of the tiny absorption band seen in the cm-1941 region [19].

Figure 3 presents the FT-IR spectrum of TAPTM-POSS, while Figure 4 shows the transmission spectrum of the applied coating. As illustrated, the POSS coating demonstrates an exceptionally high transmittance, nearly 99%, across the wavelength range of 1200 to 350 nm. At around 350 nm, the transmission curve begins to decline sharply, dropping below 15%. This steep decrease continues at shorter wavelengths. These results indicate that the coating offers excellent optical transparency within the visible spectrum, which is critical for optimal solar cell performance. At the same time, it effectively blocks harmful ultraviolet radiation, helping to prevent degradation and extend the lifespan of the solar cells. Remarkably, this high level of transmittance was achieved through careful optimization of both the coating thickness and the composite material concentration during extensive testing.

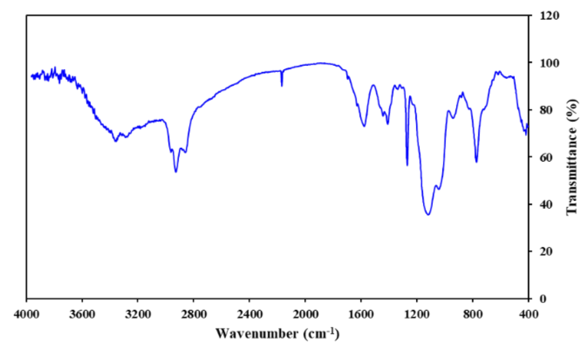

Figure 3. FT-IR spectrum related to TAPTM POSS.

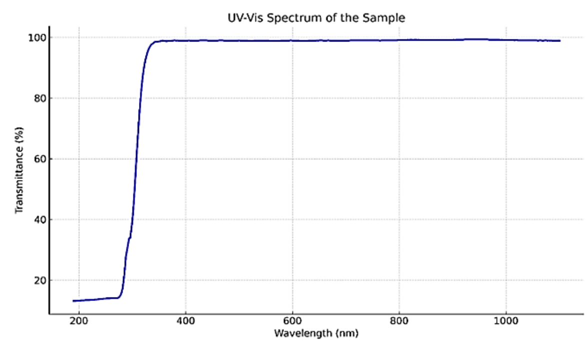

Figure 4. Transmission spectrum of the coating.

As previously stated, the pull-off test has been used to evaluate how well the coating adheres to the substrate. Three coated samples were used in this test, and Table 1 shows the analysis's findings. Following that, the data's average was reported.

Table1. pull-off test on three coated samples.

Sample No	Tensile stress psi	Mean
1	130	
2	126	128
3	128	

Following the pull-off test, the coating detached from the substrate at an average tensile stress of 128 psi (0.883 MPa). Based on these results and in accordance with ASTM D4541 and ISO 4624 standards, the coating demonstrates moderate yet acceptable adhesion to the silicon solar cell surface.

Table 2 presents the current density–voltage (J-V) characteristics of three silicone solar cell samples before and after coating with polyhedral oligomeric silsesquioxane (POSS). The data, obtained using a solar simulator integrated with a current-voltage measurement system (Figure 5), clearly demonstrate that the POSS coating consistently enhances the performance of all tested samples. Across all three samples, the power conversion efficiency (%η) increased after the coating was applied. Specifically, sample 1 exhibited an efficiency improvement from 5.083% to 5.592% (a 9.99% increase in yield), sample 2 improved from 6.754% to 7.294% (a 7.99% increase), and sample 3 increased from 4.840% to 5.330% (also a 9.99% increase). Notably, the short-circuit current density (J_{sc}) showed a consistent rise in all samples, while the fill factor (FF) and open-circuit voltage (V_{oc}) remained largely stable.

On average, the POSS coating resulted in a 9.32% relative increase in power conversion efficiency, reinforcing its effectiveness in enhancing the photovoltaic performance of the silicone-based cells. These findings confirm that surface modification via POSS contributes meaningfully to the improvement of solar cell output.

Table 2. Current density-voltage curve parameters of the samples before and after coating.

Sample type	sample	coating status	$\%\eta$	FF	V_{oc}	J_{sc}	Percentage increase in yield
Silicone cells before and after coating	1	Before coating	5.083	0.296	0.53	32.36	9.99
		After coating	5.592	0.296	0.53	35.59	
	2	Before coating	6.754	0.294	0.55	41.75	7.99
		After coating	7.294	0.294	0.55	45.09	
	3	Before coating	4.84	0.32	0.51	28.97	9.99
		After coating	5.33	0.32	0.51	31.86	

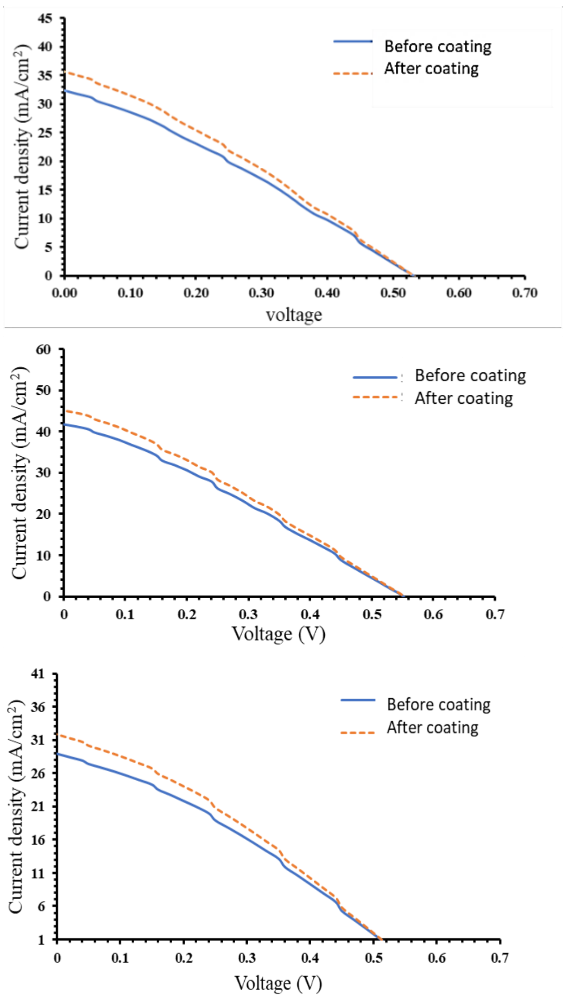

Figure 5. Current density-voltage curve of three samples of silicon solar cells before and after coating.

4. Conclusions

This study found that using POSS-based coatings with amine functional groups greatly enhanced the performance and efficiency of polycrystalline silicon solar cells. One feature of these coatings was their high optical transmittance. According to the results, POSS molecules reduced surface reflectance and improved light absorption by the solar cells (through light trapping). Therefore, the energy conversion efficiency of the polycrystalline silicon cells has increased by 9.32% without requiring any changes to their physical texture or structure. Therefore, we can conclude that POSS chemicals, as a class of surface modifiers, have a high potential to enhance solar system performance.

References

[1] D.H. Vo, A.T. Vo, Renewable energy and population growth for sustainable development in the Southeast Asian countries, Energy, Sustainability and Society 11(1) (2021) 30.

[2] G.A. Jones, K.J. Warner, The 21st century population-energy-climate nexus, Energy Policy 93 (2016) 206-212.

[3] Y. Sun, Y. Jiang, H. Wei, Z. Zhang, S. Irshad, X. Liu, Y. Xie, Y. Rui, P. Zhang, Nano-enabled strategies for greenhouse gases emission mitigation: a comprehensive review, Nano Today 57 (2024) 102378.

[4] V. Masson-Delmotte, P. Zhai, A. Pirani, S.L. Connors, C. Péan, S. Berger, N. Caud, Y. Chen, L. Goldfarb, M. Gomis, Climate change 2021: the physical science basis, Contribution of working group I to the sixth assessment report of the intergovernmental panel on climate change 2(1) (2021) 2391.

[5] S. Europe, Global market outlook for solar power 2023–2027, SolarPower Europe: Brussels, Belgium (2023).

[6] M.A. Green, E.D. Dunlop, M. Yoshita, N. Kopidakis, K. Bothe, G. Siefer, X. Hao, Solar cell efficiency tables (version 62), Progress in Photovoltaics: Research and Applications 31(7) (2023) 651-663.

[7] T.M. Razykov, C.S. Ferekides, D. Morel, E. Stefanakos, H.S. Ullal, H.M. Upadhyaya, Solar photovoltaic electricity: Current status and future prospects, Solar energy 85(8) (2011) 1580-1608.

[8] J. Jean, P.R. Brown, R.L. Jaffe, T. Buonassisi, V. Bulović, Pathways for solar photovoltaics, Energy & Environmental Science 8(4) (2015) 1200-1219.

[9] K. Alberi, J.J. Berry, J.J. Cordell, D.J. Friedman, J.F. Geisz, A.R. Kirmani, B.W. Larson, W.E. McMahon, L.M. Mansfield, P.F. Ndione, A roadmap for tandem photovoltaics, Joule 8(3) (2024) 658-692.

[10] M. Hosenuzzaman, N.A. Rahim, J. Selvaraj, M. Hasanuzzaman, A.A. Malek, A. Nahar, Global prospects, progress, policies, and environmental impact of solar photovoltaic power generation, Renewable and sustainable energy reviews 41 (2015) 284-297.

[11] A. Chatzipanagi, A. Jaeger-Waldau, S. LETOUT, A. MOUNTRAKI, B.J. GEA, A. GEORGAKAKI, E. INCE, A. SCHMITZ, Clean Energy Technology Observatory: Photovoltaics in the European Union-2024 status report on technology development, trends, value chains and markets, (2022).

[12] M. Green, E. Dunlop, J. Hohl‐Ebinger, M. Yoshita, N. Kopidakis, X. Hao, Solar cell efficiency tables (version 57), Progress in photovoltaics: research and applications 29(1) (2021) 3-15.

[13] A. Goodrich, P. Hacke, Q. Wang, B. Sopori, R. Margolis, T.L. James, M. Woodhouse, A wafer-based monocrystalline silicon photovoltaics road map: Utilizing known technology improvement opportunities for further reductions in

manufacturing costs, Solar Energy Materials and Solar Cells 114 (2013) 110-135.

[14] B.V. Stefani, M. Kim, Y. Zhang, B. Hallam, M.A. Green, R.S. Bonilla, C. Fell, G.J. Wilson, M. Wright, Historical market projections and the future of silicon solar cells, Joule 7(12) (2023) 2684-2699.

[15] G.A. Barron-Gafford, M.A. Pavao-Zuckerman, R.L. Minor, L.F. Sutter, I. Barnett-Moreno, D.T. Blackett, M. Thompson, K. Dimond, A.K. Gerlak, G.P. Nabhan, Agrivoltaics provide mutual benefits across the food–energy–water nexus in drylands, Nature Sustainability 2(9) (2019) 848-855.

[16] S. Wei, Y. Chen, Z. Zeng, An unexpectedly large proportion of photovoltaic facilities installed on cropland, The Innovation Energy 2(1) (2025) 100070-1-100070-3.

[17] T. He, R. Yang, W. Xiao, Y. Ye, Y. Hu, Y. Chen, Z. Sun, K. Wang, W. Chen, M. Zhang, Trading Food for Energy? Global Evidence of Solar Projects Undermining Food Security, (2024).

[18] K. Ghani, N. Kiomarsipour, M. Ranjbar, New high-efficiency protective coating containing glycidyl-POSS nanocage for improvement of solar cell electrical parameters, Journal of Nanostructures 9(1) (2019) 103-111.

[19] I. Jerman, A.Š. Vuk, M. Koželj, F. Švegl, B. Orel, Influence of amino functionalised POSS additive on the corrosion properties of (3-glycidoxypropyl) trimethoxysilane coatings on AA 2024 alloy, Progress in Organic Coatings 72(3) (2011) 334-342.