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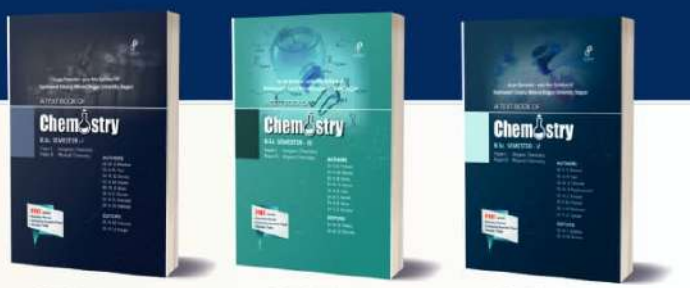

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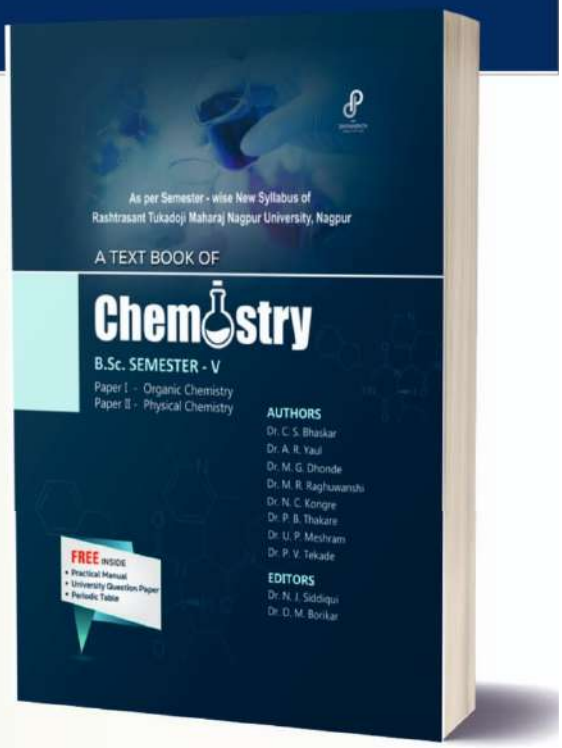

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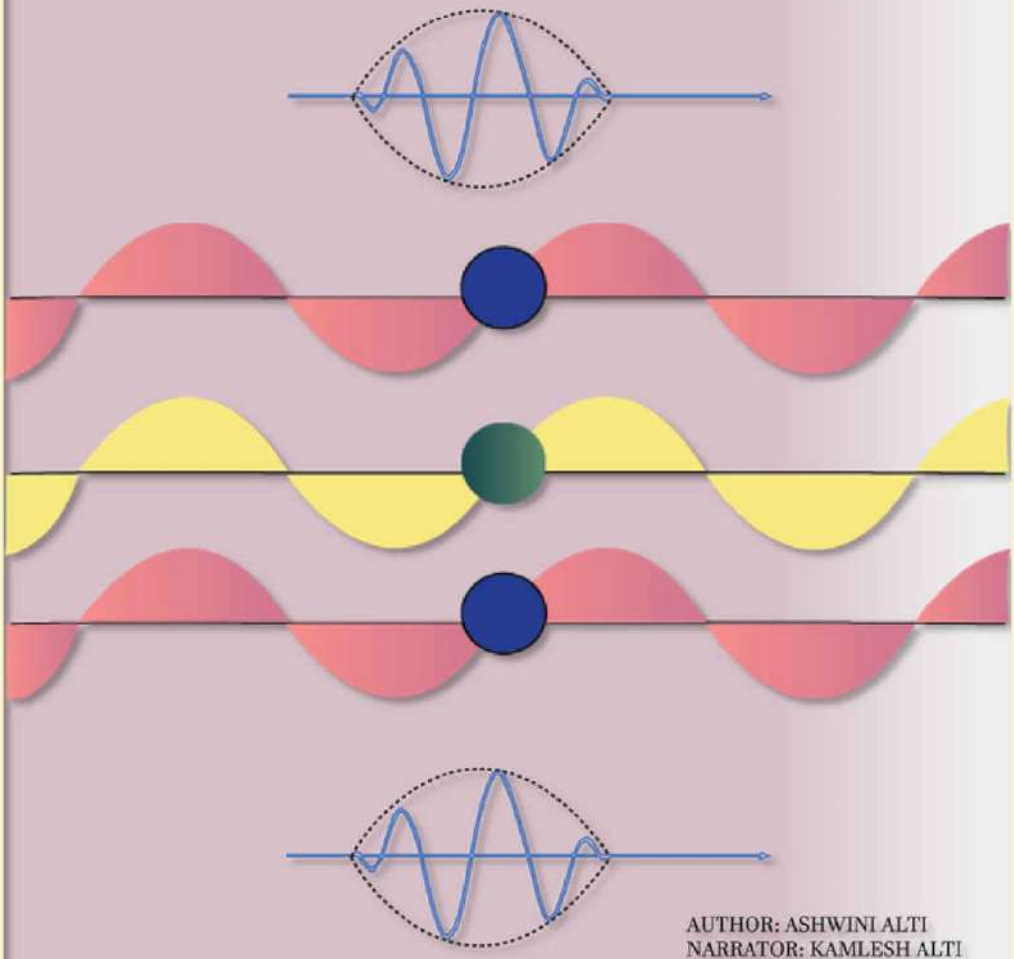

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Abstract

In present chapter we have reported green and highly efficient method for synthesize novel series of substituted -1H-indazol-3-amine derivative (3a-h) by cyclocondensation reaction of substituted benzonitrile (1a-h) and substituted Hydrazine (2a-h) using ceric (IV) ammonium nitrate (CAN) as a catalyst, EtOH-H2O as a ecofriendly media and reaction was carried out under ultrasound irradiation green method. The structures of newly synthesized indazole derivative (3a-h) were corroborated through spectral investigation such as elemental analysis and spectral studies like IR, C13 NMR, Mass spectra and 1H NMR. The compounds were assessed for their in-vitro antimicrobial activity with pathogenic microbe comprising Gram positive bacterial strains, S. aureus and Gram negative strains E.coli, P.vulgaris, and S. typhi at di erent concentration. The consequence of bioassay is compared with standard drug Chloramphenicol.

Keywords

indazol | ceric (IV) ammonium nitrate catalyst | ultrasound irradiation | ecofriendly media | antimicrobial screening

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1. Introduction

Indazole was first defined as a “pyrazole ring fused with the benzene ring” by the scientist Emil Fisher. It is broadly studied due to its remarkable chemical and biological properties. Indazole is from the azoles family containing carbon, hydrogen and nitrogen atoms. Indazole also called as benzpyrazole or isoindazolone which containing two nitrogen atoms. It is ten π-electron aromatic heterocyclic systems as a pyrazole molecule. The structure of indazole is given below in cylindrical bonds is as ( ).

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DOI: 10.5772/intechopen.81269

WRITTEN BY

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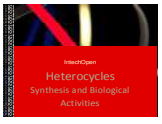

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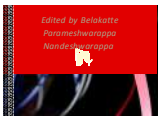

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Abstract

Pharmaceutics and therapeutics industries enforced chemists to seek/discover antibacterial novel heterocycles owing specific bioactivity and innate characteristics significance. This chapter summarized potent antibacterial profile of 5-oxo-imidazolines in the new millennium as an antibacterial against Gram-positive and Gram-negative bacteria viz. B. thuringiensis, S. aureus, E. coli, and E. aerogenes is presented in this chapter. 5-(H/Br benzofuran-2-yl)-1-phenyl 1H-pyrazole-3-carbohydrazides are condensed with 4-(arylidene)-2 phenyloxazol-5(4H)-one in acetic acid at elevated temperature to yield product 5-(H/Br benzofuran-2-yl)-N-(4-arylidene-5-oxo-2-phenyl-4,5-dihydroimidazol-1-yl)-1-phenyl-1H-pyrazole-3-carboxamides. Di erent substrates like 4-(arylidene)-2-phenyloxazol-5(4H)-one allowed to react with benzaldehyde hippuric acid to yield 5-oxo-imidazolines/5-oxo-4,5-dihydroimidazole. All synthesized 5-oxo-imidazolines were characterized via elemental analysis and FT-IR, 1H-NMR and mass spectra techniques. All 5-oxo-imidazolines assayed in vitro for inherent antimicrobial activity at di erent concentration against stated bacterial strains and compared with standard chloramphenicol. 5-Oxo-imidazolines (3a and 3c) with 125 µg/mL concentration showed excellent antibacterial profile against Gram-positive bacteria, B. thuringiensis, while other derivatives at di erent concentrations showed moderate antibacterial activity against Gram-positive bacteria, S. aureus and B. thuringiensis. Gram-negative bacteria like E. coli and E. aerogenes are tested at higher concentration (1000, 500, and 125 µg/mL) and found good-to-moderate antibacterial activity. Tested products found non-active against E. aerogenes for 125, 61, and 31 µg/mL concentration also inactive at conc. 31 µg/mL against E. coli.

Keywords

antibacterial | Gram positive/negative | B. thuringiensis | S. aureus | E. coli | E. aerogenes | 5-oxo-imidazoline | azlactones | medicinal

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Chapter sections

1. Introduction

Imidazole is a planer five-member ring with molecular formula $C_3N_2H_4$, containing three carbon atoms and two nitrogen atoms in 1 and 3 skeletal positions as depicted in . This is an aromatic heterocyclic ring that's classified as a diazole family owing non-adjacent nitrogens in its skeleton.

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Dr. Naqui Jahan Siddiqui
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Institute of Science, Nagpur

Five and Six Membered Heterocycles: Synthesis, Characterization and Their Antimicrobial and Antioxidant Activities

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Authors: Mohammad Idrees and Naqui Jahan Siddiqui

CHAPTER

12

Li-S ion batteries: a substitute for Li-ion storage batteries

Kalpana R. Nagde[1], *S.J. Dhoble*[2]

[1]Department of Physics, Institute of Science, Nagpur, Maharashtra, India; [2]Department of Physics, RTM Nagpur University, Nagpur, Maharashtra, India

Introduction

After the discovery of electricity, there was a need to find effective methods to store energy for use on demand. A device that stores energy is known as an accumulator or battery. Different forms of energy are available in nature, which include radiation energy, electricity, gravitational potential energy, chemical energy, and kinetic energy. Energy storage also involves converting energy from different forms to more conveniently storable forms. There are some technologies that store energy for a short period, while others can store it for longer. Some examples of energy storage devices are the rechargeable battery, hydroelectric dam, fossil fuel storage, and mechanical, electrical, biological, electrochemical, thermal, and chemical storage devices. During the 20th century, electricity was generated by burning fossil fuel. Due to pollution from fossil fuels, researchers have concentrated their attention on renewable energy sources like solar and wind energy [1]. At the beginning of 21st century, portable devices were in demand all over the world. In this chapter, attention is given to electrochemical devices, which include batteries.

Energy storage materials

Materials for chemical and electrochemical energy storage are key for a diverse range of applications, including batteries, hydrogen storage, sunlight conversion into fuels, and thermal energy storage. The urgent need for energy storage materials for a sustainable and carbon-free society is the main stimulant for the new dawn in the development of functional materials for energy storage and conversion. Hydride-based all-solid-state batteries, which are considered to be safer, cheaper, and more abundant, while potentially having higher

Energy Materials
https://doi.org/10.1016/B978-0-12-823710-6.00008-X

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Proceedings of the 15th Annual IEEE International
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TDDFT Studies on Sheet Size-Dependency of Optoelectronic Properties of 2D Silicon Doped with Alkali Metals

MD Raiyan Alam, Muath Bani Salim, *Student Member, IEEE,* Ganesh Alwarappan, Aashka Bhandari, Sunil Patil, Sherin Alfalah, Mohamed Shibl, Walid Hassan, Reza Nekovei, *Senior Member, IEEE*, and Amit Verma, *Senior Member, IEEE*

Abstract—This work investigates the effect of alkali metals (Li, Na, and K) doping on silicene sheets (2D silicon) by using Time-Dependent Density Functional Theory (TDDFT). This includes $Si_{13}H_{22}$, $Si_{19}H_{30}$, $Si_{54}H_{74}$, and $Si_{104}H_{134}$ silicene sheets. The results show some variation in the IR and UV-Vis spectrums as the sheet size change, with the largest structure showing an onset of absorption in the visible spectrum. Also, the results show that excitation energy decreases significantly by 29% as the number of atoms increases from $Si_{13}H_{22}$to $Si_{104}H_{134.}$ Also, this work investigates the doping effect of alkali metals (Li, Na, and K) on the silicene sheets. The doped structures showed a dipole moment as high as approximately 10 Debye. The doped structures show a significant increase in optical absorption in the visible spectrum, as well as the potential for high reactivity

I. Introduction

Silicene has a similar honeycomb band structure like graphene and potentially shows stronger coupling between the internal layer and higher oxidation resistance than graphene [1], [2]. Besides that, the Silicene energy gap can be tuned by doping alkali atoms or by an electric field, and it has high Fermi velocity and carrier mobility [3], [4]. On the other hand, more intense spin-orbit coupling, and compatibility with current Si fabrication are various other advantages over graphene [5]. Therefore, the novel two-dimensional material; silicene, has recently gained extensive popularity attracting both theoretical and experimental studies by different research communities. So far, chemists have been able to produce silicene sheets and nanoribbons depending on silver, iridium, diboride thin films [6]. The ambipolar current-voltage relationship has been reported in silicene material [7]. Another study shows the interaction of silicene with non-metallic surfaces based on density functional theory (DFT) [7]. The effects of the electronic properties of silicene in presence with alkali metal atom absorption are synthesized [7]. At present, researchers expect silicene to possess an enormous potential for application in technology over graphene [8].

In silicene, each Si atom is bonded with three more Si atoms, forming a honeycomb lattice, like graphene, or germanene. In this work, four hydrogen-terminated structures were considered with the increasing number of Si atoms. The first part of the investigation investigates the optoelectronic properties of the pristine structures. The rest of this study investigates the effects of doping the structures with alkali metals, Li, Na, and K. This was motivated by the recent importance of the Si-Alkali Metal (AM) systems. Li-Si system is being considered for Lithium–silicon batteries. Lithium–silicon batteries are a lithium-ion battery technology that employs a silicon anode and lithium ions as the charge carriers [9]. Na-Si system is considered for hydrogen production as sodium silicate is a reducing agent [10], while the K-Si system serves as a corrosion inhibitor (reducing the rate of corrosion) [11]. Replacing bulk Si with 2D silicon sheets in the above applications may have the potential to increase reactivity and efficiency because of the greater surface-to-volume ratio afforded by 2D sheets.

This paper is structured as follows; Section 2 describes the proposed computational details and the applied methodology of the TDDFT. Results for the performance of dipole moments, UV, and IR spectra are presented in Section 3. Summary and conclusions at the ends

J. Computational Details

TDDFT simulation is used to analyze the electronic properties of four different Silicene, by B3LYP functional and 6-31G (d) basis set [12], [13]. The simulation is done with the help of the Gaussian 16 program [14], and it covers the following Silicene structures $Si_{13}H_{22}$, $Si_{19}H_{30}$, $Si_{54}H_{74}$, and $Si_{104}H_{134}$. The chosen 6-31G (d) basis set is to add more flexibility to account for the asymmetry about the nucleus.

Firstly, optimized molecular structures are required before any TDDFT simulation. Then the vibrational frequencies are calculated for the Silicene structures. Also, the TDDFT is used to evaluate the Silicene's oscillator strength values and obtain the absorption spectrum in the Ultraviolet-visible (UV-VIS) region, which is required to find the amount of energy that the material can absorb [15].

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K. RESULTS

The top and side view of the optimized structures are shown in Figs. 1(a) and 1(b). Figure 2 shows the onset of a small distortion from the ideal free-standing structure for the largest structure silicone structure considered in this work.

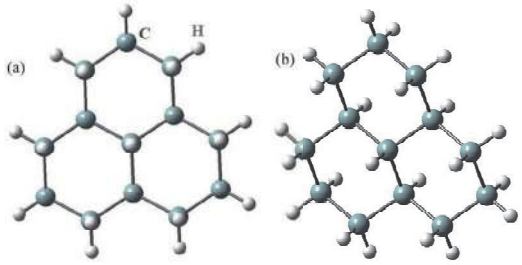

Figure 1. (a) Top view of the molecular structure of Si $_3H_{22}$ showing honeycomb lattice (b) 3D view of Si $_3H_{22}$ showing two vertically displaced sub-lattices

While Fig. 2 shows the structure doped with Li the distortion is present in pristine structures too. This observed distortion is seen to be relatively smaller than one reported for germanene, the 2D Germanium sheets [16].

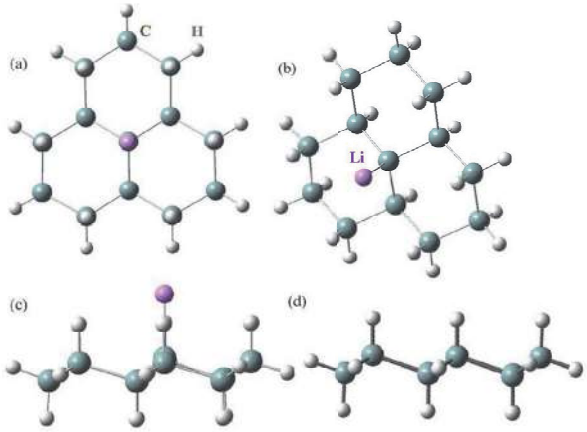

Figure 2. (a) Top view of the molecular structure of $Si_{13}H_{22}$ with Li doping (b) 3D view of $Si_{13}H_{22}$ with Li doping (c) Side view of $Si_{13}H_{22}$ with Li doping (d) Side view of undoped $Si_{13}H_{22}$

The mass-weighted coordinates method is used to find the vibrational frequencies or the infrared (IR) spectrum for the Silicene structures as shown in Fig.3 [17]. The IR spectrum in Fig. 3 represents the molar absorptivity coefficient (S) in $Mole^{-1}$ cm^{-1} vs. wavenumber in cm^{-1}. The results show that $Si_{13}H_{22}$ has a band frequency of fewer than 75.5 cm^{-1}, and the Si-H out of plane bending vibration frequencies is between 600-900 $cm^{-1,}$ which is very close to the reported experimental frequency of 620 cm^{-1}. Also, the 75.6-150 cm^{-1} frequency range is for the Si-H in-plane bending vibration. Likewise, the peak vibration frequency in Fig.3 is around 600-800 cm^{-1}, and the Si-H stretching vibration is 2125-2245 cm^{-1} ,which is very close to the experimental values in [18].

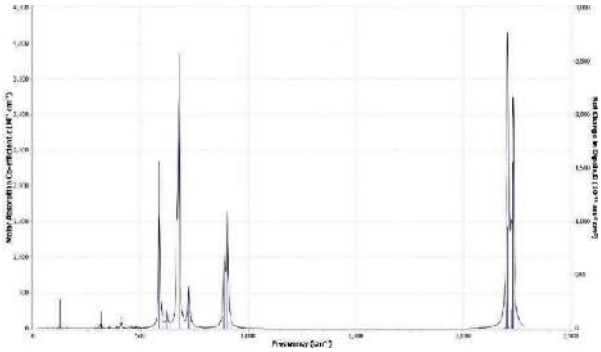

Figure 3. (a) IR spectrum of Si13H22.

The absorption spectrum for Silicene structures is calculated by convolving the oscillator strength values that are obtained from the TFDFT simulation, as shown in Fig. 4.

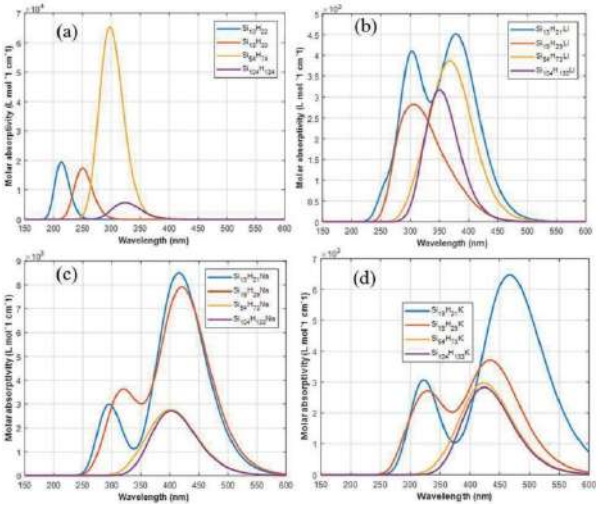

Figure 4. Molar Absorption (a) Undoped, (b) Li doping, (c) Na doping (d) K doping

Figure 5 shows the density of states (DOS) spectrum for pristine, Li-, Na-, and K-doped Si104H133 sheets. The bandgap from DOS shows no significant change across the four structures. Similar observations were also made for the other structures with an equal number of Si atoms.

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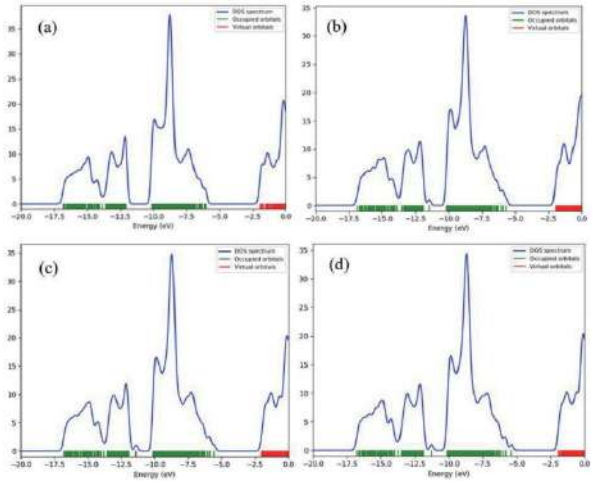

Figure 5. (a) Density of States spectrum for (a) $Si_{104}H_{134}$, (b) $Si_{104}H_{133}Li$, (c) $Si_{104}H_{133}Na$ and (d) $Si_{104}H_{133}K$.

Table I shows the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), and the HOMO-LUMO bandgap E_g for the Silicene structures in this study. The alkali metals lower the bandgap for the all of the silicene sheets in this study, as also mentioned in [18][19] for other 2D sheets, making them suitable for wide range of applications like LEDs and lasers.

TABLE I. SILICENE ENERGY LEVELS

	HOMO (eV)	LUMO (eV)	Eg (eV)
$Si_{13}H_{22}$	-6.95	-1.02	5.94
$Si_{13}H_{21}Li$	-5.84	-1.83	4.01
$Si_{13}H_{21}Na$	-5.58	-2.14	3.44
$Si_{13}H_{21}K$	-5.15	-2.00	3.14
$Si_{19}H_{30}$	-6.63	-1.35	5.28
$Si_{19}H_{29}Li$	-5.55	-1.46	4.09
$Si_{19}H_{29}Na$	-5.38	-1.98	3.40
$Si_{19}H_{29}K$	-5.19	-1.80	3.39
$Si_{54}H_{74}$	-6.15	-1.86	4.29
$Si_{54}H_{73}Li$	-5.94	-1.93	4.01
$Si_{54}H_{73}Na$	-5.55	-1.92	3.63
$Si_{54}H_{73}K$	-5.33	-1.86	3.47
$Si_{104}H_{134}$	-6.03	-1.93	4.10
$Si_{104}H_{133}Li$	-5.68	-1.97	3.71
$Si_{104}H_{133}Na$	-5.58	-1.96	3.62
$Si_{104}H_{133}K$	-5.38	-1.91	3.47

Table II lists the calculated dipole moments for the doped and pristine sheets. As it can be observed from this table, the doped sheets have significantly larger dipole moments, with the Li-doped sheets being comparable to reported values for Li-doped graphene sheets [20]. K-doped sheets have dipole moment values comparable to Na [21]. It is observed that dipole moment values decrease for doped sheets with increasing the number of Si atoms. This may be attributed to the increased influence of the Si sheets, which reduces the effects of the dopant.

TABLE II. DIPOLE MOMENT OF DIFFERENT SIZED & DOPED STRUCTURES.

Number of Si Atoms	Doped Li (Debye)	Doped Na (Debye)	Doped K (Debye)	Undoped (Debye)
13	5.9217	6.6988	9.7637	0.1074
19	4.1539	5.6431	8.6511	0.1065
54	5.8206	5.4398	8.0859	0.2145
104	5.2362	6.3355	8.8415	0.6248

L. CONCLUSION

The optoelectronic properties for different sizes of Silicene have been studied in this work. The results show that as the sheet size increases Silicene will have a stronger absorption spectrum than bulk or nanowire silicon. Silicon may remain the lead material in the optoelectronic and electronic applications. The work also suggests that doped silicone sheets may have significant potential in many advanced applications, including Li-ion batteries.

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Mangrove – Interesting Group of Plants

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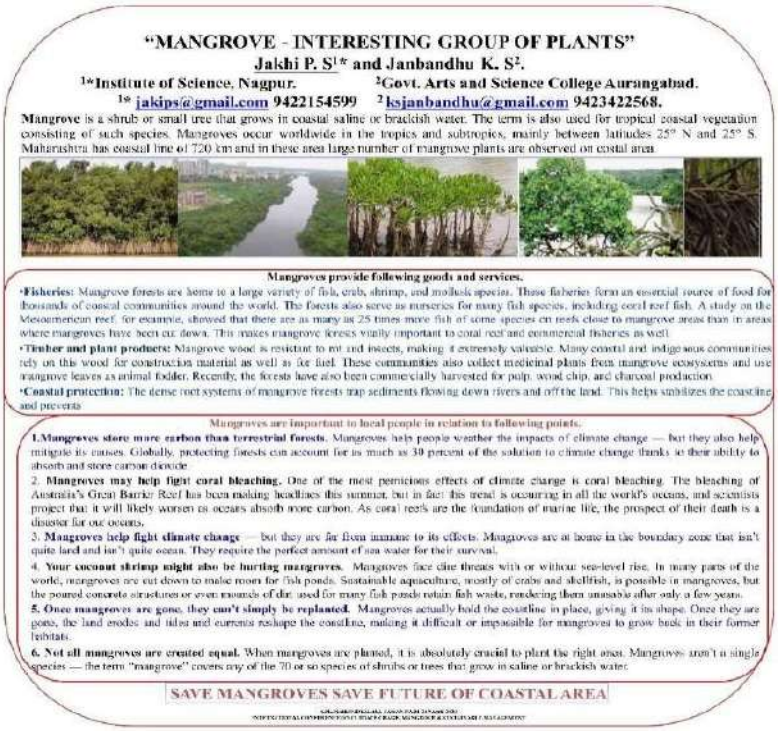
Abstract Mangroves are very interesting and important group of plants from coastal area. Maharashtra is one of the important state of India having coastal area of about 720 km. Large population of Mangroves available in the coastal area of Mumbai City, Mumbai Suburban, Thane, Palghar, Raigad, Ratnagiri and Sindhudurg. Many more peoples are not aware regarding the important role of mangrove in their life. Mangroves play very crucial role in the livelihood of this area by keeping this view in mind various aspects of mangrove enlisted in the poster. It will be awareness activity regarding mangrove in community.

Poster



"MANGROVE - INTERESTING GROUP OF PLANTS"

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Mangrove is a shrub or small tree that grows in coastal saline or brackish water. The term is also used for tropical coastal vegetation consisting of such species. Mangroves occur worldwide in the tropics and subtropics, mainly between latitudes 25° N and 25° S. Maharashtra has coastal line of 720 km and in these area large number of mangrove plants are observed on costal area.

Mangroves provide following goods and services.

•**Fisheries:** Mangrove forests are home to a large variety of fish, crab, shrimp, and mollusk species. These fisheries form an essential source of food for thousands of coastal communities around the world. The forests also serve as nurseries for many fish species, including coral reef fish. A study on the Mesoamerican reef, for example, showed that there are as many as 25 times more fish of some species on reefs close to mangrove areas than in areas where mangroves have been cut down. This makes mangrove forests vitally important to coral reef and commercial fisheries as well.

•**Timber and plant products:** Mangrove wood is resistant to rot and insects, making it extremely valuable. Many coastal and indigenous communities rely on this wood for construction material as well as for fuel. These communities also collect medicinal plants from mangrove ecosystems and use mangrove leaves as animal fodder. Recently, the forests have also been commercially harvested for pulp, wood chip, and charcoal production.

•**Coastal protection:** The dense root systems of mangrove forests trap sediments flowing down rivers and off the land. This helps stabilizes the coastline and prevents

Mangroves are important to local people in relation to following points.

1.**Mangroves store more carbon than terrestrial forests.** Mangroves help people weather the impacts of climate change — but they also help mitigate its causes. Globally, protecting forests can account for as much as 30 percent of the solution to climate change thanks to their ability to absorb and store carbon dioxide.

2. **Mangroves may help fight coral bleaching.** One of the most pernicious effects of climate change is coral bleaching. The bleaching of Australia's Great Barrier Reef has been making headlines this summer, but in fact this trend is occurring in all the world's oceans, and scientists project that it will likely worsen as oceans absorb more carbon. As coral reefs are the foundation of marine life, the prospect of their death is a disaster for our oceans.

3. **Mangroves help fight climate change** — but they are far from immune to its effects. Mangroves are at home in the boundary zone that isn't quite land and isn't quite ocean. They require the perfect amount of sea water for their survival.

4. **Your coconut shrimp might also be hurting mangroves.** Mangroves face dire threats with or without sea-level rise. In many parts of the world, mangroves are cut down to make room for fish ponds. Sustainable aquaculture, mostly of crabs and shellfish, is possible in mangroves, but the poured concrete structures or even mounds of dirt used for many fish ponds retain fish waste, rendering them unusable after only a few years.

5. **Once mangroves are gone, they can't simply be replanted.** Mangroves actually hold the coastline in place, giving it its shape. Once they are gone, the land erodes and tides and currents reshape the coastline, making it difficult or impossible for mangroves to grow back in their former habitats.

6. **Not all mangroves are created equal.** When mangroves are planted, it is absolutely crucial to plant the right ones. Mangroves aren't a single species — the term "mangrove" covers any of the 70 or so species of shrubs or trees that grow in saline or brackish water.

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