

# Photoluminescence in a Glucose-coated Sila-fullerane and Its Nanomedicine Applications

Mohammad Qasemnazhand

University of Zanjan

Farhad Khoeini (✉ [khoeini@znu.ac.ir](mailto:khoeini@znu.ac.ir))

Department of Physics, University of Zanjan, P.O. Box 45195-313, Zanjan, Iran

Farah Marsusi

Amirkabir University of Technology

---

## Research Article

**Keywords:** Sila-dodecahedron, Photoluminescence, Nano-bait, Density functional theory, Cancer cells

**Posted Date:** January 27th, 2021

**DOI:** <https://doi.org/10.21203/rs.3.rs-152222/v1>

**License:** © ⓘ This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

---

# Photoluminescence in a glucose-coated sila-fullerane and its nanomedicine applications

Mohammad Qasemnazhand<sup>1</sup>, Farhad Khoeini<sup>1\*</sup>, Farah Marsusi<sup>2</sup>

<sup>1</sup>*Department of Physics, University of Zanjan, P.O. Box 45195-313, Zanjan, Iran*

<sup>2</sup>*Department of Physics, Amirkabir university of technology, P.O. Box 15875-4413, Tehran, Iran*

\*Corresponding author's email: [khoeini@znu.ac.ir](mailto:khoeini@znu.ac.ir)

## ABSTRACT

In this study, we introduce nano-baits that are formed based on the binding of glucose in a silicon nanoparticle. Sila-dodecahedrane has been selected among of four other famous nanostructures, due to its high stability, biocompatibility and its ability to engineer electronic features. Because of the glucose attached to nano-baits, they are attractive to cancer cells that consume high glucose. In this research, two nano-baits have been modeled with the chemical formulas of  $\text{Si}_{20}\text{H}_{19}\text{C}_6\text{H}_{11}\text{O}_6$  and  $\text{Si}_{20}\text{H}_{13}(\text{C}_6\text{H}_{11}\text{O}_6)_7$ . Their optimal structures are obtained using density functional theory (DFT). For this, we use the B3LYP hybrid functional and 6-31+g(d,p) basis set. Vibration frequency calculations show that the glucose binding of a sila-dodecahedrane has a stable bond. These nano-baits with photoluminescence determine the location of cancer cells. By adjusting the number of glucoses attached to these nano-baits, the energy required for their excitation and light response can be adjusted. These nano-baits are a viable alternative to radioactive materials for locating cancer cells.

**Keywords:** Sila-dodecahedron, Photoluminescence, Nano-bait, Density functional theory, Cancer cells.

## 1. Introduction

Although surgery, chemotherapy, and radiotherapy are traditional and commonly used treatments for cancer, new methods such as antibodies, antigens, and photodynamic therapy have been proposed. Understanding the physiological characteristics and physiological roles of human cells will lead to an appropriate approach to solve biological problems. For example, the Photodynamic therapy method uses a photo sensitizer substance. By injection of Photo Sensitizer into the patient, this substance is accumulated in the cancerous tumor. To detect and treat illness, ultraviolet and red-light radiations are used, respectively. It can be said about the mechanism of photo sensitizer delivery to the tumor that they have Low-density lipoprotein (LDL) cholesterol receptors for example neoplastic materials, such as hydrophobic porphyrin. Since cancerous cells are associated with severe cell division, LDLs consume more than normal, so they need a lot of LDL and absorb it, therefore, by covering PS in the porphyrin, the chance of PS reaching the mass increases [1-4].

In this research, we focus on other characteristics of cancer cells. Cancer cells have higher glucose consumption than other cells in the body [5-6]. So this can give us a new idea at least for detecting the location of cancer cells, if we design nanoparticles that glucose molecules connected it, then these nanoparticles act as nano-baits. Now, if these nano-baits are injected into the patient's body, they accumulate in the tumor, and the cancer cells are detected by photoluminescence [7-8].

To identify the appropriate nanoparticles, first we investigate chemically and optically the fullerene, fullerane molecules and silicon analogues. Finally, we identified silicon structures as a good candidate for optical cancer detection, because in addition to its biodegradability and biodegradability [9-10], due to proper derivatization we expect the desired photoluminescence.

## 2. Computational Method

In this research, we use density functional theory method to investigate the structural features and stability of structures. We obtain the optimal structures and calculate the total energies with DFT. The B3LYP, the hybrid function that also includes the Hartree-Fock (HF) method, describes the interaction between atoms in our calculations, and for describing the orbitals shapes, we used split valence and polarized basis set that assembled in the form 6-31+g(d,p). Finally, our calculations are performed by using of Gaussian software [11-14].

## 3. Results

We first obtain the electrochemical properties of the structures introduced in the introduction, Buckminster fullerene, smallest fullerene, dodecahedrane, and sila-dodecahedrane. The schematic of these structures is shown in figure 1.

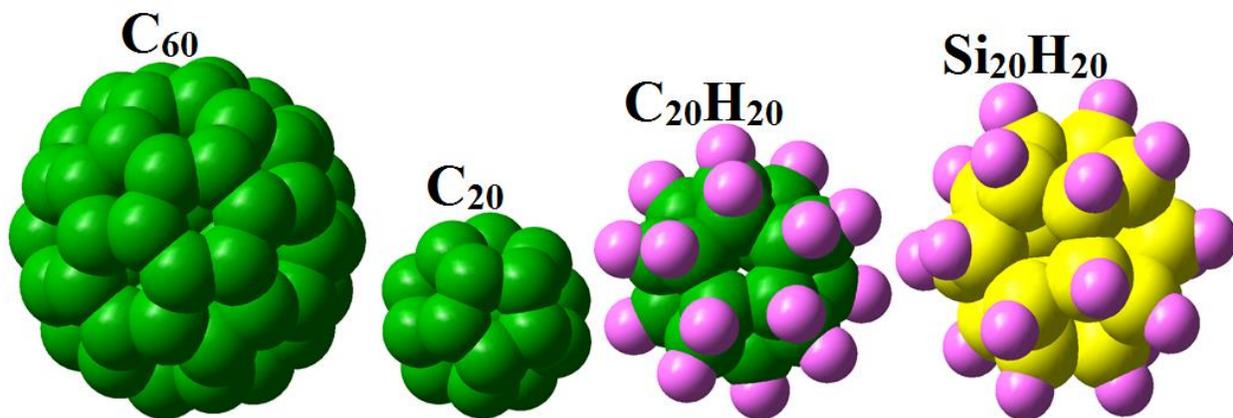


Figure 1. Candidate structures to design nano-baits.

For this, we obtain HOMO and LUMO energy levels with DFT calculations. Now, using the following equations, we can obtain electronic properties, such as HOMO-LUMO gap, chemical potential, chemical hardness, and the estimate of electron affinity [15-17]:

$$E_{Gap} = E_{LUMO} - E_{HOMO}. \quad (1)$$

$$\mu = \frac{(E_{HOMO} + E_{LUMO})}{2}. \quad (2)$$

$$\eta = \frac{(E_{HOMO} - E_{LUMO})}{2}. \quad (3)$$

$$EA = -E_{LUMO}. \quad (4)$$

The new index, electrophilicity, can be obtained using chemical potential and chemical hardness through equation 5. With regard to this index, the difference between the two structures can be seen better [18].

$$\omega = \frac{\mu^2}{2\eta}. \quad (5)$$

For the studied structures, we calculate the above electronic properties. The values are given in Table 1.

Table 1. A list of some of the electronic features of the studied structures (in unit eV).

Structures	HOMO	LUMO	E <sub>Gap</sub>	μ	η	EA	ω
C <sub>60</sub>	-6.40	-3.68	2.72	-5.04	1.36	3.68	9.32
C <sub>20</sub>	-5.51	-3.61	1.89	-4.56	0.95	3.61	10.97
C <sub>20</sub> H <sub>20</sub>	-7.24	-0.19	7.04	-3.71	3.52	0.19	1.96
Si <sub>20</sub> H <sub>20</sub>	-6.83	-2.36	4.48	-4.60	2.24	2.36	4.72

Our first choice, to design a nano-bait was using C<sub>60</sub>, the fullerene molecule. Because a lot of research has suggested the fullerene molecule for tumor targeting, and the treatment of cancer [19-26]. However, the reported toxicity to fullerenes prevents work on this molecule, and this causes us to remove this molecule from our choices [27-29]. Its low chemical hardness and high electron affinity, confirms the toxicity of fullerene.

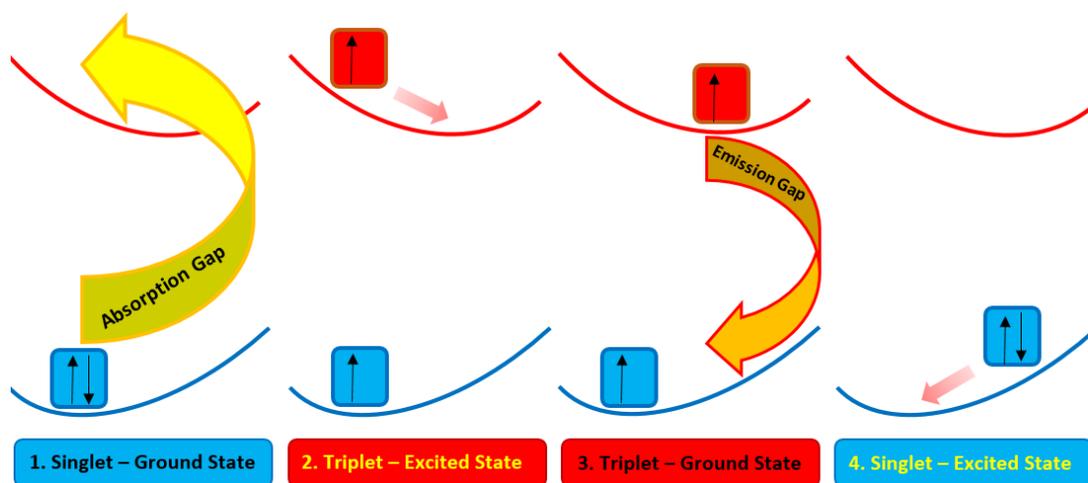
To increase the chemical hardness, we can consider the quantum confinement effect (QCE). As the size of the nanoparticles decreases, the energy gap increases due to the QCE, with the help of interpretation of the particle in the box [30-32]. For this reason, instead of C<sub>60</sub> fullerene, we use the smallest fullerene, C<sub>20</sub>. But the smallest fullerene, the C<sub>20</sub>, has not stable structure [33-34]. Our results, such as low chemical hardness and high electrophilicity, confirm this. But with the saturation of its structure, everything changes.

When the C<sub>20</sub> structure is saturated with hydrogen, the Dodecahedrane, with the chemical formula C<sub>20</sub>H<sub>20</sub>, is formed. In 1982, Leo Paquette et al. succeeded in synthesizing this symmetric

molecule [35]. Dodecahedrane has the highest chemical hardness and the lowest electron affinity and electrophilicity, among the studied structures, according to our results given in Table 1. Since the selective structure is ultimately located in the biological environment, we are interested in examining the silicon analog of dodecahedrane as well as it is known as biocompatibility and biodegradability. We obtain interesting features for the sila-dodecahedrane. Sila-dodecahedrane has a stable structure so that even its chemical hardness is higher than  $C_{60}$  fullerene, but despite having a structure saturated with hydrogen, it also has high electron affinity and electrophilicity. It should be noted that in 2015, Wagner et al. synthesized silicon dodecahedrane as a sila-fullerene with an endohedral chloridelon [36].

Dodecahedrane and its silicon analogue are two candidate structures of the four introduced structures. But to determine which carbon or silicon structures can provide the desired optoelectronic properties, we dop their surfaces with functional groups containing oxygen. Since we want to attach the glucose molecule to the nanoparticle, we must choose a functional group that can be compared to glucose. To do this, we have chosen the hydroxyl functional group, which in addition to its binding site is similar to the glucose molecule, also has a smaller number of atoms, which reduces the computational cost in DFT.

Now, we can calculate the optical absorption gap for pure and functionalized structures by subtracting the total energy of the optimized-ground state from the total energy of the excited state at the same geometry as the ground state, as shown in figure 2.



**Figure 2. The absorption and emission gaps of the system. Above schematic shows the cause of the absorption and emission gap differences in the nanoparticles.**

Because the number of electrons of the  $X_{20}Y_{20}$  is even, its spin state will be singlet, in the ground state. The lower-energy triplet excited-state is optically inactive, according to the  $\Delta S=0$  selection rule. Therefore, the lowest-energy allowed optical transition excites the system into the singlet excited state [37-39].

The energy of the singlet excited state is higher than the triplet state, due to larger repulsive coulomb interactions between antiparallel spins. Therefore, the excited system may relax from

the singlet state into the triplet one. Therefore, we calculate the emission bandgap from the relaxed excited triplet state to the ground state at the same energy, as shown in figure 2. Using equations 6 and 7, the absorption and emission gap can be obtained:

$$Gap_{\text{Absorption}} = E_{\text{Triplet}}^{\text{Exited}} - E_{\text{Singlet}}^{\text{Ground}} \quad (6)$$

$$Gap_{\text{Emission}} = E_{\text{Triplet}}^{\text{Ground}} - E_{\text{Singlet}}^{\text{Exited}} \quad (7)$$

Finally, the difference between the absorption and emission gaps shows the stoke shift:

$$\Delta E_{\text{Stoke Shift}} = Gap_{\text{Absorption}} - Gap_{\text{Emission}} \quad (8)$$

We present the calculated absorption and emission gaps of the desired structure in Table 2.

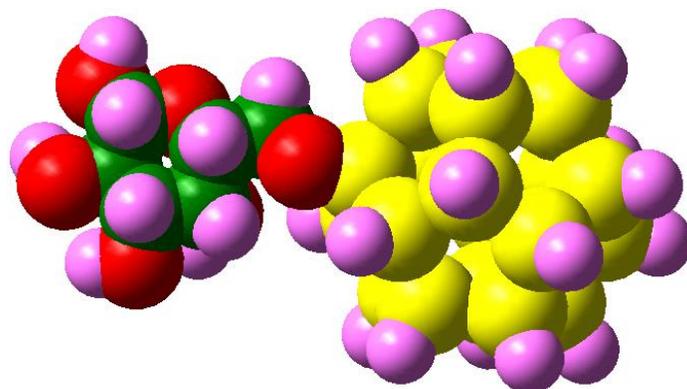
Table 2. A list of the electronic and optoelectronic gaps of the studied structures (in unit eV).

Structures	HOMO	LUMO	H-L Gap	Absorption Gap	Emission Gap	Stoke Shift
<b>C<sub>20</sub>H<sub>20</sub></b>	-7.24	-0.19	7.04	6.34	5.83	0.51
<b>C<sub>20</sub>(OH)<sub>20</sub></b>	-7.41	-2.14	5.27	4.48	3.99	0.49
<b>Si<sub>20</sub>H<sub>20</sub></b>	-6.83	-2.36	4.48	3.71	3.32	0.39
<b>Si<sub>20</sub>(OH)<sub>20</sub></b>	-5.90	-3.82	2.08	1.37	0.63	0.74

The data given in Table 2 clearly presents the two results. First, Optical gaps are smaller than HOMO-LUMO gaps, and second, silicon structures are more engineered electrical and electro-optical than carbon structures. These results are consistent with our previous researches [40-41]. More important than the above results, it is the emission gap of sila-dodecahedrane by suitable functionalized can be to reach the visible or even infrared range. While the dodecahedrane gives an ultraviolet response due to ultraviolet stimulating.

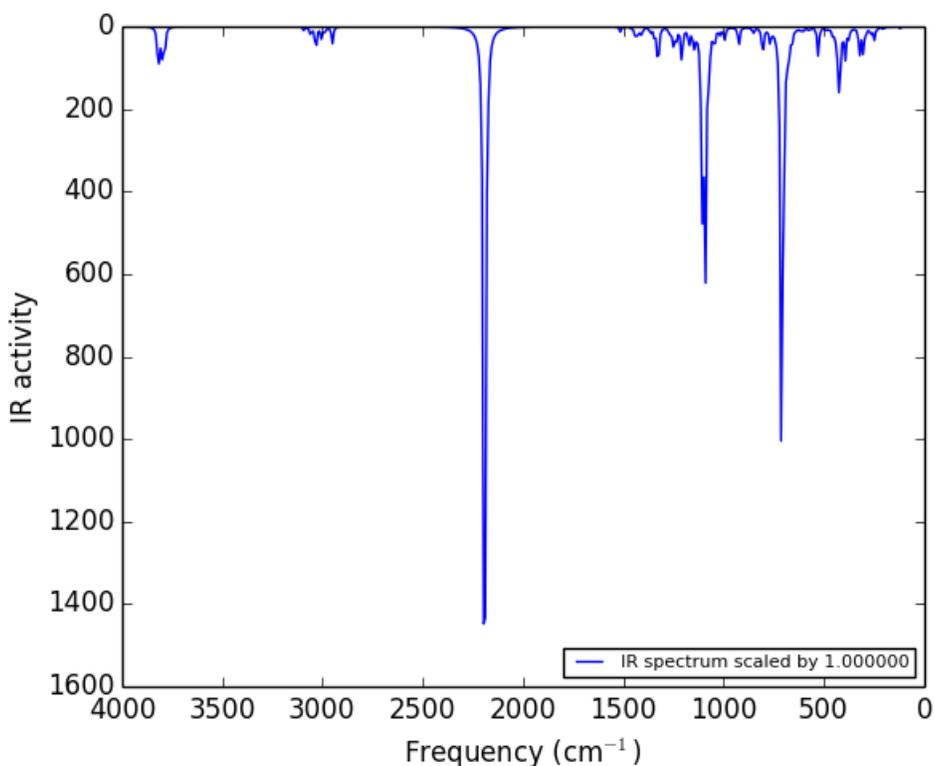
Since silicon nanoparticles are known for their biocompatibility, their infrared response due to their ultraviolet stimulating can be used in thermotherapy [42]. The visible response can also be used to detect cancer cells, but to do, these particles must be attractive to cancer cells.

Now we have to make sila-dodecahedrane functionalized in such a way that in addition to visible response to ultraviolet stimulating, it must also be an attractive bait for cancer cells. To do this, as mentioned earlier, we use the trick of attaching a glucose molecule to Sila-dodecahedrane. Since cancer cells consume a lot of glucose, our nanoparticles will act as nano-bait for them. In Figure 3. you can see a model of the desired nano-bait.



**Figure 3. A labeled sila-dodecahedrane with glucose acts as a nano-bait.**

It should be noted that the frequency calculations of introduced nano-bait do not have a negative frequency, i.e. the structure do not contain imaginary vibrations, so this structure is at the minimum level in the energy diagram and is stable [43]. Figure 4. Shows the infrared spectrum diagram for the introduced nano-bait.



**Figure 4. The infrared spectrum of a labeled sila-dodecahedrane with glucose, that acts as a nano-bait.**

Table 3. Contains the energies of the structure of pure and glucose-labeled sila-dodecahedrane in the ground and excited states. By calculating the energy required to transfer the structure from the ground state to the excited state, adiabatically, we obtain the absorption gap. Besides, calculating the difference of the excited structure energy in optimal geometry with the energy of

singlet state in the same geometry, we get the emission gap. Based on the data given in Table 3, we can conclude that our nano-bait is excited by UV-A rays and gives a visible response with indigo blue light.

Table 3. The absorption and emission gaps for the  $\text{Si}_{20}\text{H}_{20}$  and its glucose-labeled structure (in unit eV).

Nanoparticle & nano-bait	Singlet (Ground)	Triplet (Adiabatic)	Absorption gap	Singlet (Adiabatic)	Triplet (Ground)	Emission Gap	Stokes shift
$\text{Si}_{20}\text{H}_{20}$	-157889.48	-157885.77	3.71	-157889.26	-157885.94	3.32	0.39
$\text{Si}_{20}\text{H}_{19}\text{C}_6\text{H}_{11}\text{O}_6$	-176552.05	-176548.81	3.24	-176549.06	-176551.74	2.68	0.56

The data in Table 2 show that we can conclude that by adding the number of glucoses attached to the sila-dodecahedrane, it is possible to excite the nano-bait even with less energetic light. Of course, with the same argument, we can conclude that it will respond with light with longer wavelengths too. In the following, another nano-bait with more glucose is introduced, you can see its model in Figure 5.

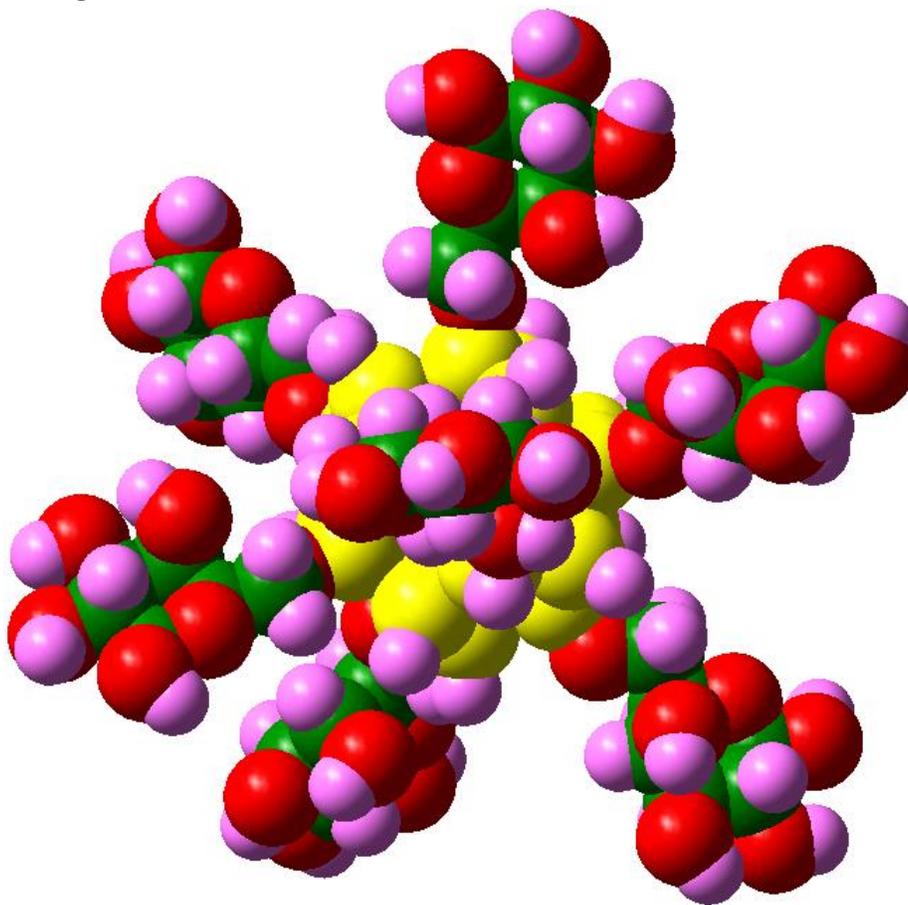


Figure 5. Dodecahedrane based silicon nano-bait surrounded by seven glucose molecules attached to it.

Figure. 5. shows  $\text{Si}_{20}\text{H}_{13}(\text{C}_6\text{H}_{11}\text{O}_6)_7$ , a nano-bait formed by the binding of seven glucose molecules to a sila-dodecahedrane. Our calculations show that the absorption gap of this nano-bait is about

2.57 eV, and its emission gap is about 2.06 eV. As we expected, according to the procedure in Table 3, as the number of glucoses attached to the nanoparticles increases, the energy required for excitation also decreases, and the optical response shifts to longer wavelengths. Therefore, with proper functionalized, even the response of these nanoparticles reaches the infrared range, in which case, these nanoparticles can also be used for thermotherapy.

The size of the nanoparticles shown in figure 5 are about 2 nanometers. Note that, it is not necessary for nano-baits to be sila-dodecahedrane based, because silicon nanoparticles with sizes of 1 to 2 nm, have similar chemical properties. This also reduces the production costs of these nanoparticles [44-45].

#### **4. Conclusion**

In this research, we introduced nano-baits that are formed based on the binding of glucose in sila-dodecahedrane. These nanoparticles, because of the glucose attached to them, are attractive to cancer cells that consume high glucose, and they can be used as bait. By adjusting the number of glucoses attached to these nanoparticles, the energy required for their excitation and light response can be adjusted. These nano-baites can be a good alternative to methods of detecting cancer cell or even treating that have high costs and side risks.

#### **DATA AVAILABILITY**

All data generated for this study are included in the article.

#### **AUTHOR CONTRIBUTIONS**

M. Qasemnazhand carried out the simulations, analyzed the data and prepared the manuscript. F.K. supervised the project and revised the final manuscript. F. marsusi supported DFT calculations. All authors read and approved the final manuscript.

**Competing interests:** The authors declare no competing interests.

#### **Acknowledgments**

The authors gratefully acknowledge Ali Ghaemi, a hard-working physician, for his guidance on the idea of the work.

## References and Notes

1. Ormond, Alexandra, and Harold Freeman. "Dye sensitizers for photodynamic therapy." *Materials* **6**, 3 (2013).
2. Fukuda, Haydée, Adriana Casas, and Alcira Batlle. "Aminolevulinic acid: from its unique biological function to its star role in photodynamic therapy." *The international journal of biochemistry & cell biology* **37**, 2 (2005).
3. Novo, Mercedes, Gereon Hüttmann, and Heyke Diddens. "Chemical instability of 5-aminolevulinic acid used in the fluorescence diagnosis of bladder tumours." *Journal of Photochemistry and Photobiology B: Biology* **34**,2 (1996).
4. Khalkhali, M., Mohammadinejad, S., Khoeini, F., & Rostamizadeh, K. (2019). Vesicle-like structure of lipid-based nanoparticles as drug delivery system revealed by molecular dynamics simulations. *International Journal of Pharmaceutics*, 559, 173-181.
5. DeBerardinis, Ralph J., Nabil Sayed, Dara Ditsworth, and Craig B. Thompson. "Brick by brick: metabolism and tumor cell growth." *Current opinion in genetics & development* **18**, 1 (2008).
6. Wise, David R., and Craig B. Thompson. "Glutamine addiction: a new therapeutic target in cancer." *Trends in biochemical sciences* **35**, 8 (2010).
7. Erogbogbo, Folarin, Chen-An Tien, Ching-Wen Chang, Ken-Tye Yong, Wing-Cheung Law, Hong Ding, Indrajit Roy, Mark T. Swihart, and Paras N. Prasad. "Bioconjugation of luminescent silicon quantum dots for selective uptake by cancer cells." *Bioconjugate chemistry* **22**, 6 (2011).
8. Geng, Bijiang, Dewen Yang, Dengyu Pan, Liang Wang, Fengfeng Zheng, Wenwen Shen, Chen Zhang, and Xiaokai Li. "NIR-responsive carbon dots for efficient photothermal cancer therapy at low power densities." *Carbon* **134**, 153, (2018).
9. Park, J. H., Gu, L., Von Maltzahn, G., Ruoslahti, E., Bhatia, S. N., & Sailor, M. J. (2009). Biodegradable luminescent porous silicon nanoparticles for in vivo applications. *Nature materials*, 8(4), 331.
10. Romero, J. J., Llansola-Portolés, M. J., Dell'Arciprete, M. L., Rodríguez, H. B., Moore, A. L., & Gonzalez, M. C. (2013). Photoluminescent 1–2 nm sized silicon nanoparticles: a surface-dependent system. *Chemistry of Materials*, 25(17), 3488-3498.
11. Lee, C.; Yang, W.; Parr, RG. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B.* **1988**, 37, 785.
12. Petersson, GA.; Malick, DK.; Wilson, WG.; Ochterski, JW.; Montgomery, Jr JA.; Frisch, MJ. Calibration and comparison of the Gaussian-2, complete basis set, and density functional methods for computational thermochemistry. *J. Chem. Phys.* **1998**, 109, 10570-10579.
13. Hehre, W. J., Ditchfield, R., & Pople, J. A. Self-consistent molecular orbital methods. XII. Further extensions of Gaussian-type basis sets for use in molecular orbital studies of organic molecules. *The Journal of Chemical Physics*. 1972, 56(5), 2257-2261.
14. Ditchfield, R. H. W. J., Hehre, W. J., & Pople, J. A. Self-consistent molecular-orbital methods. IX. An extended Gaussian-type basis for molecular-orbital studies of organic molecules. *The Journal of Chemical Physics*, 1971, 54(2), 724-728.
15. Wang, T., Lu, J., Zhu, H., Liu, J., Lin, X., Liu, Y., & Tang, Y. The electronic properties of chiral silicon nanotubes. *Superlattices and Microstructures*. 2017, 109, 457-462.

16. Tavakol, H., & Shahabi, D. DFT, QTAIM, and NBO study of adsorption of rare gases into and on the surface of sulfur-doped, single-wall carbon nanotubes. *The Journal of Physical Chemistry C*. 2015, 119(12), 6502-6510.
17. Zhan, C. G., Nichols, J. A., & Dixon, D. A. Ionization potential, electron affinity, electronegativity, hardness, and electron excitation energy: molecular properties from density functional theory orbital energies. *The Journal of Physical Chemistry A*. 2003, 107(20), 4184-4195.
18. Qasemnazhand, M., Khoeini, F., & Marsusi, F. (). Fulleryne, a new member of the carbon cages family. arXiv preprint arXiv. 2020, 2003.09835.
19. Zhang, Q., Yang, W., Man, N., Zheng, F., Shen, Y., Sun, K., Li, Y. and Wen, L.P., 2009. Autophagy-mediated chemosensitization in cancer cells by fullerene C60 nanocrystal. *Autophagy*, 5(8), pp.1107-1117.
20. Shi, J., Wang, L., Gao, J., Liu, Y., Zhang, J., Ma, R., Liu, R. and Zhang, Z., 2014. A fullerene-based multi-functional nanoplatform for cancer theranostic applications. *Biomaterials*, 35(22), pp.5771-5784.
21. Wang, H., Agarwal, P., Zhao, S., Yu, J., Lu, X. and He, X., 2016. Combined cancer therapy with hyaluronan-decorated fullerene-silica multifunctional nanoparticles to target cancer stem-like cells. *Biomaterials*, 97, pp.62-73.
22. Shi, J., Wang, B., Wang, L., Lu, T., Fu, Y., Zhang, H. and Zhang, Z., 2016. Fullerene (C60)-based tumor-targeting nanoparticles with "off-on" state for enhanced treatment of cancer. *Journal of Controlled Release*, 235, pp.245-258.
23. Zogovic, N.S., Nikolic, N.S., Vranjes-Djuric, S.D., Harhaji, L.M., Vucicevic, L.M., Janjetovic, K.D., Misirkic, M.S., Todorovic-Markovic, B.M., Markovic, Z.M., Milonjic, S.K. and Trajkovic, V.S., 2009. Opposite effects of nanocrystalline fullerene (C60) on tumour cell growth in vitro and in vivo and a possible role of immunosuppression in the cancer-promoting activity of C60. *Biomaterials*, 30(36), pp.6940-6946.
24. Davydenko, M.O., Radchenko, E.O., Yashchuk, V.M., Dmitruk, I.M., Prylutsky, Y.I., Matishevskaya, O.P. and Golub, A.A., 2006. Sensibilization of fullerene C60 immobilized at silica nanoparticles for cancer photodynamic therapy. *Journal of molecular liquids*, 127(1-3), pp.145-147.
25. Guan, M., Ge, J., Wu, J., Zhang, G., Chen, D., Zhang, W., Zhang, Y., Zou, T., Zhen, M., Wang, C. and Chu, T., 2016. Fullerene/photosensitizer nanovesicles as highly efficient and clearable phototheranostics with enhanced tumor accumulation for cancer therapy. *Biomaterials*, 103, pp.75-85.
26. Maleki, R., Khoshoei, A., Ghasemy, E. and Rashidi, A., 2020. Molecular insight into the smart functionalized TMC-Fullerene nanocarrier in the pH-responsive adsorption and release of anti-cancer drugs. *Journal of Molecular Graphics and Modelling*, 100, p.107660.
27. Usenko, C.Y., Harper, S.L. and Tanguay, R.L., 2007. In vivo evaluation of carbon fullerene toxicity using embryonic zebrafish. *Carbon*, 45(9), pp.1891-1898.
28. Johnston, H.J., Hutchison, G.R., Christensen, F.M., Aschberger, K. and Stone, V., 2010. The biological mechanisms and physicochemical characteristics responsible for driving fullerene toxicity. *Toxicological Sciences*, 114(2), pp.162-182.

29. Sayes, C.M., Marchione, A.A., Reed, K.L. and Warheit, D.B., 2007. Comparative pulmonary toxicity assessments of C60 water suspensions in rats: few differences in fullerene toxicity in vivo in contrast to in vitro profiles. *Nano letters*, 7(8), pp.2399-2406.
30. Norris, DJ.; Bawendi, MG. Measurement and assignment of the size-dependent optical spectrum in CdSe quantum dots. *Phys. Rev. B*. **1996**, 53,16338.
31. Smilowitz, L.; McBranch, D.; Klimov, V.; Robinson, JM.; Koskelo, A.; Grigorova, M.; Mattes, BR.; Wang, H.; Wudl, F. Enhanced optical limiting in derivatized fullerenes. *Opt. Lett.* **1996**, 21, 922-924.
32. Pietryga, JM.; Park, YS.; Lim, J.; Fidler, AF.; Bae, WK.; Brovelli, S.; Klimov, VI. Spectroscopic and device aspects of nanocrystal quantum dots. *Chem. Rev.* **2016**, 116, 10513-10622.
33. Rad, Ali Shokuhi, Sadegh Mehdi Aghaei, Elahe Aali, and Majid Peyravi. "Study on the electronic structure of Cr-and Ni-doped fullerenes upon adsorption of adenine: a comprehensive DFT calculation." *Diamond and Related Materials* 77 (2017): 116-121.
34. Matolepsza, E., Witek, H. A., & Irle, S. (2007). Comparison of geometric, electronic, and vibrational properties for isomers of small fullerenes C20– C36. *The Journal of Physical Chemistry A*, 111(29), 6649-6657.
35. Ternansky, R. J., Balogh, D. W., & Paquette, L. A. (1982). Dodecahedrane. *Journal of the American Chemical Society*, 104(16), 4503-4504.
36. Tillmann, J., Wender, J. H., Bahr, U., Bolte, M., Lerner, H. W., Holthausen, M. C., & Wagner, M. One-Step Synthesis of a [20] Silafullerane with an Endohedral Chloride Ion. *Angewandte Chemie International Edition*. 2015, 54(18), 5429-5433.
37. Patrick, C. E., & Giustino, F. Quantum nuclear dynamics in the photophysics of diamondoids. *Nature communications*. 2013, 4, 2006.
38. Marsusi, F. Nuclear dynamic effects on electronic properties of functionalized diamondoids. *Physica E: Low-dimensional Systems and Nanostructures*. 2018, 103, 435-443.
39. Marsusi, F., J. Sabbaghzadeh, and N. D. Drummond. "Comparison of quantum Monte Carlo with time-dependent and static density-functional theory calculations of diamondoid excitation energies and Stokes shifts." *Physical Review B* 84.24 (2011): 245315.
40. Hong, C., Lee, J., Zheng, H., Hong, S. S., & Lee, C. (2011). Porous silicon nanoparticles for cancer phototherapy. *Nanoscale research letters*, 6(1), 321.
41. Qasemnazhand, M., Khoeini, F., & Shekarforoush, S. Electronic transport properties in the stable phase of a cumulene/B 7/cumulene molecular bridge investigated using density functional theory and a tight-binding method. *New Journal of Chemistry*. 2019, 43(42), 16515-16523.
42. Marsusi, F., & Qasemnazhand, M. Sila-fulleranes: promising chemically active fullerene analogs. *Nanotechnology*. 2016, 27(27), 275704.
43. Li, J., Bai, H., Yuan, N., Wu, Y., Ma, Y., Xue, P., & Ji, Y. (2014). Density functional theory studies of Si36H36 and C36H36 nanocages. *International Journal of Quantum Chemistry*, 114(11), 725-730.
44. Qasemnazhand, M, and Marsusi, F, "Theoretical Study of Opto-Electronic properties of Silafulleranes Using Density Functional Theory." (2018): 77-87.

45. Romero, J. J., Llansola-Portolés, M. J., Dell’Arciprete, M. L., Rodríguez, H. B., Moore, A. L., & Gonzalez, M. C. (2013). Photoluminescent 1–2 nm sized silicon nanoparticles: a surface-dependent system. *Chemistry of Materials*, 25(17), 3488-3498.

# Figures



Figure 1

Candidate structures to design nano-baits.

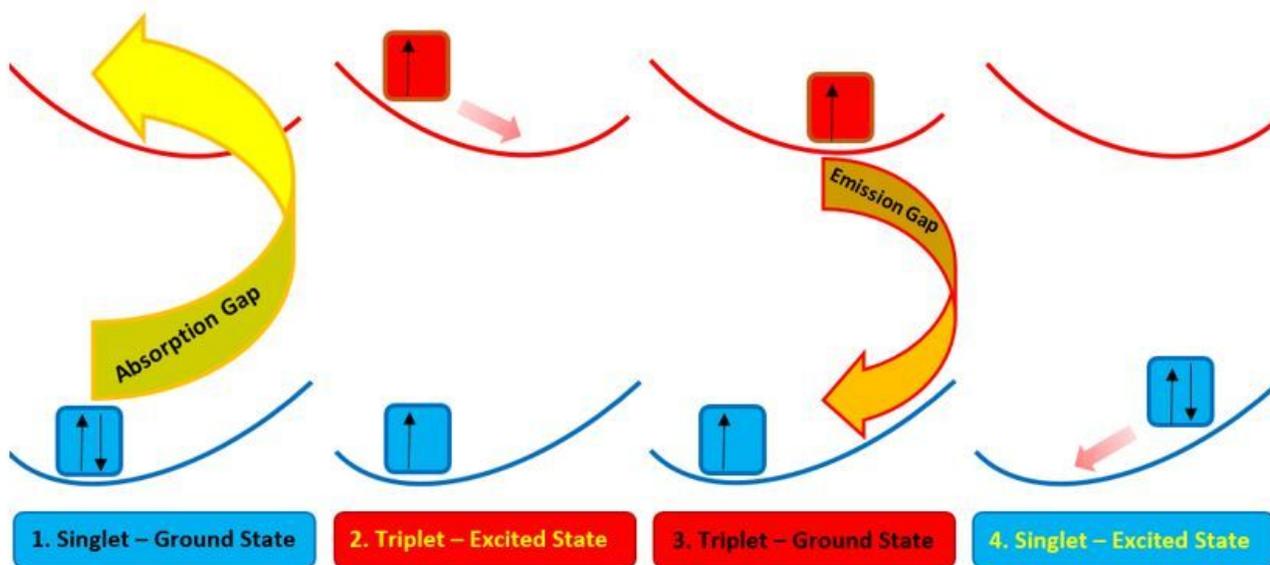
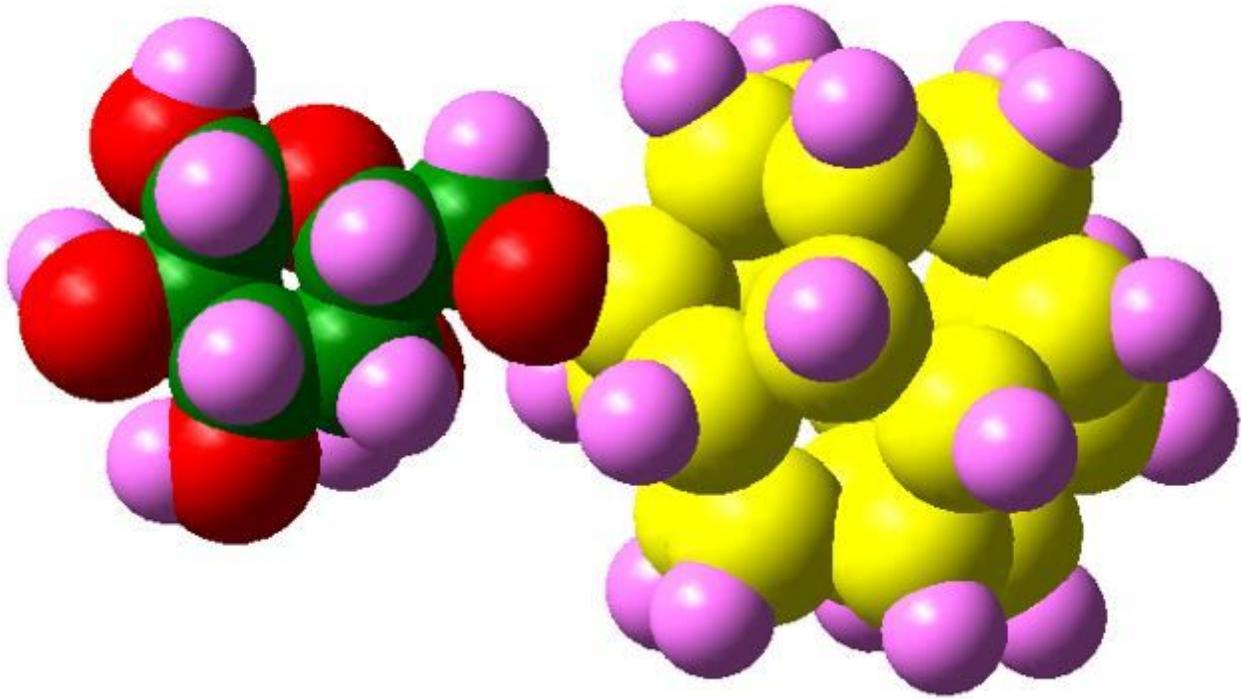


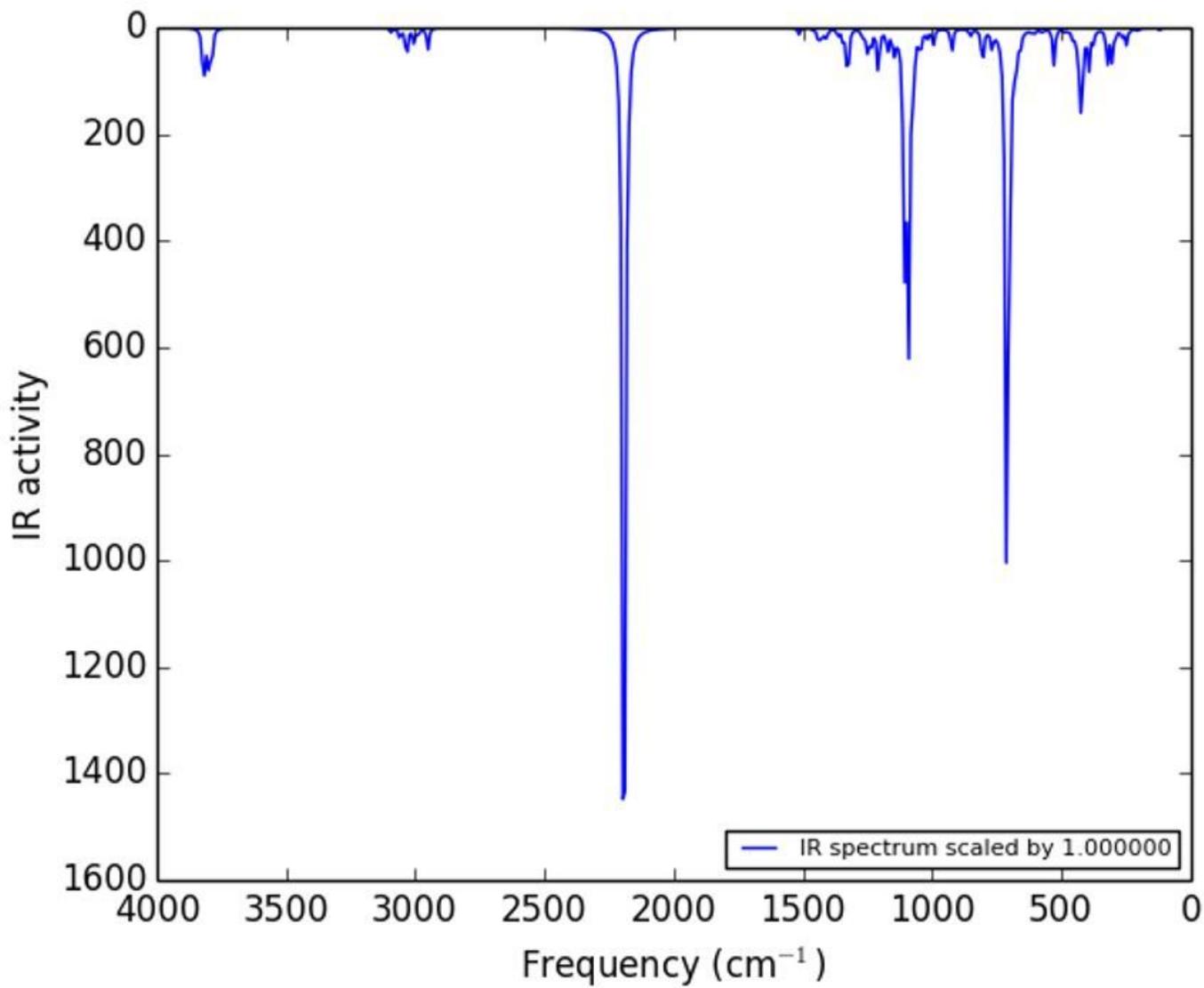
Figure 2

The absorption and emission gaps of the system. Above schematic shows the cause of the absorption and emission gap differences in the nanoparticles.



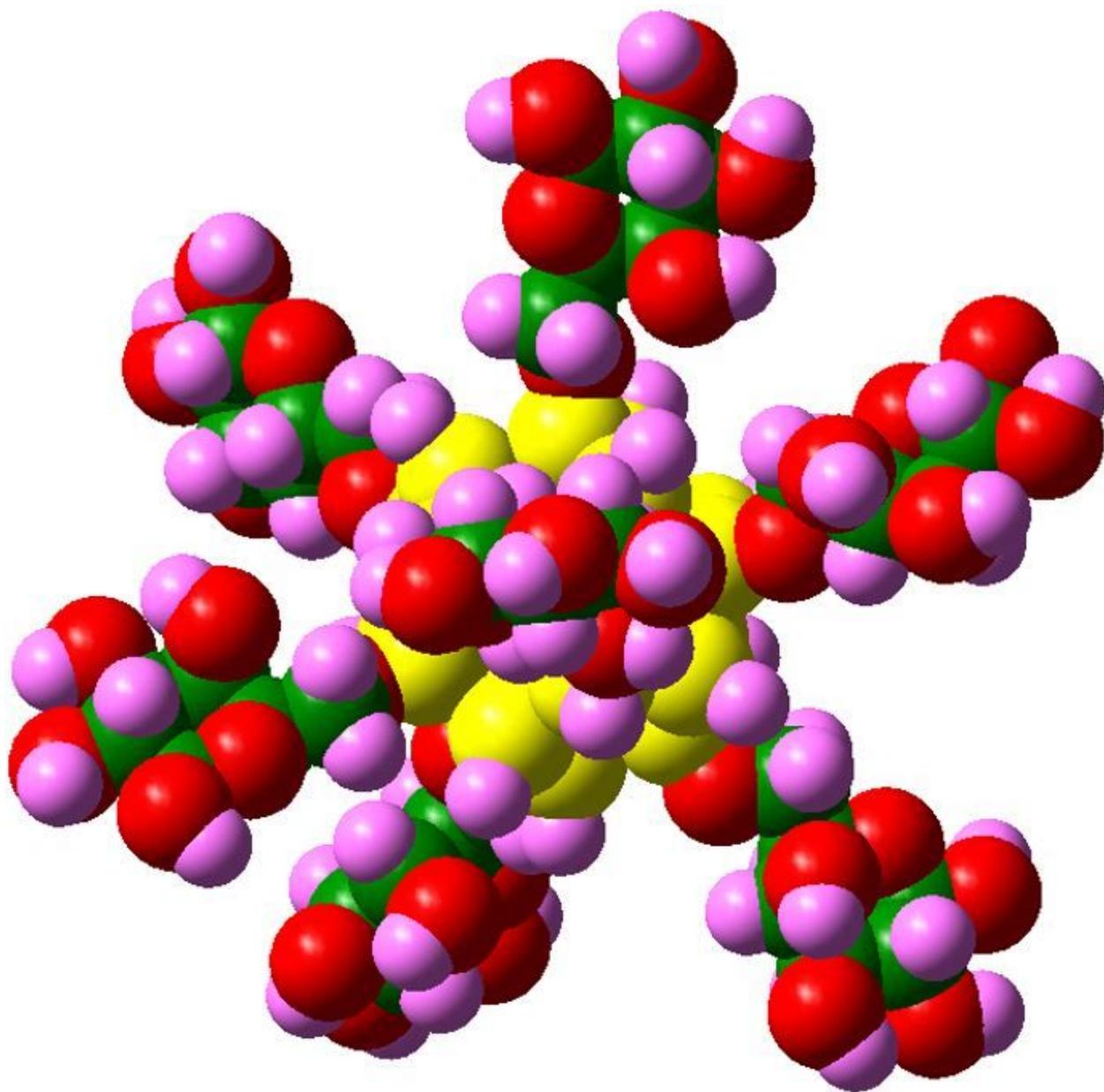
**Figure 3**

A labeled sila-dodecahedrane with glucose acts as a nano-bait.



**Figure 4**

The infrared spectrum of a labeled sila-dodecahedrane with glucose, that acts as a nano-bait.



**Figure 5**

Dodecahedrane based silicon nano-bait surrounded by seven glucose molecules attached to it.