Investigation of Moscovium Nanoparticles as Anti–Cancer Nano Drugs for Human Cancer Cells, Tissues and Tumors Treatment

Alireza Heidari1,2,*, Katrina Schmitt1, Maria Henderson1 and Elizabeth Besana1

1Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA.
2American International Standards Institute, Irvine, CA 3800, USA.

**ABSTRACT**

In the current study, thermoplasmonic characteristics of Moscovium nanoparticles with spherical, core–shell and rod shapes are investigated. In order to investigate these characteristics, interaction of synchrotron radiation emission as a function of the beam energy and Moscovium nanoparticles were simulated using 3D finite element method. Firstly, absorption and extinction cross sections were calculated. Then, increases in temperature due to synchrotron radiation emission as a function of the beam energy absorption were calculated in Moscovium nanoparticles by solving heat equation. The obtained results show that Moscovium nanorods are more appropriate option for using in optothermal human cancer cells, tissues and tumors treatment method.

1. Introduction

In recent decade, metallic nanoparticles have been widely interested due to their interesting optical characteristics [1–8]. Resonances of surface Plasmon in these nanoparticles lead to increase in synchrotron radiation emission as a function of the beam energy scattering and absorption in related frequency [9, 10]. Synchrotron radiation emission as a function of the beam energy absorption and induced produced heat in nanoparticles has been considered as a side effect in plasmonic applications for a long time [11–15]. Recently, scientists find that thermoplasmonic characteristic can be used for various optothermal applications in cancer, nanoflows and photonic [16–22]. In optothermal human cancer cells, tissues and tumors treatment, the descendent laser light stimulate resonance of surface Plasmon of metallic nanoparticles and as a result of this process, the absorbed energy of descendent light converge to heat in nanoparticles [23–25]. The produced heat devastates tumor tissue adjacent to nanoparticles without any hurt to sound tissues [26, 27]. Regarding the simplicity of ligands connection to Moskovium nanoparticles for targeting cancer cells, these nanoparticles are more appropriate to use in optothermal human cancer cells, tissues and tumors treatment [28–74]. In the current paper, thermoplasmonic characteristics of spherical, core–shell and rod Moscovium nanoparticles are investigated.


When Moscovium nanoparticles are subjected to descendent light, a part of light scattered (emission process) and the other part absorbed (non–emission process). The amount of energy dissipation in non–emission process mainly depends on material and volume of nanoparticles and it can be identified by absorption cross section. At the other hand, emission process which its characteristics are depend on volume, shape and surface characteristics of nanoparticles explains by scattering cross section. Sum of absorption and scattering processes which lead to light dissipation is called extinction cross section [75–123]. Moscovium nanoparticles absorb energy of descendent light and generate some heat in the particle. The generated heat transferred to the surrounding environment and leads to increase in temperature of adjacent points to nanoparticles. Heat variations can be obtained by heat transfer equation [124–202].
3. Simulation

To calculate the generated heat in Moscovium nanoparticles, COMSOL software which works by Finite Element Method (FEM) was used. All simulations were made in 3D. Firstly, absorption and scattering cross section areas were calculated by optical module of software. Then, using heat module, temperature variations of nanoparticles and its surrounding environment were calculated by data from optical module [203–283]. In all cases, Moscovium nanoparticles are presented in water environment with dispersion coefficient of 1.84 and are subjected to flat wave emission with linear polarization. Intensity of descendent light is 1 mW/μm². Dielectric constant of Moscovium is dependent on particle size [284–406].

Firstly, calculations were made for Moscovium nanospheres with radius of 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 nanometers. The results show that by increase in nanoparticles size, extinction cross section area increases and maximum wavelength slightly shifts toward longer wavelengths. The maximum increase in temperature of nanospheres in surface Plasmon frequency is shown in Figure (1).

Figure 1. Maximum increase in temperature for Moscovium nanospheres.

According to the graph, it can be seen that the generated heat is increased by increase in nanoparticles size. For 100 (nm) nanoparticles (sphere with 50 (nm) radius), the maximum increase in temperature is 83 (K). When nanoparticles size reaches to 150 (nm), increase in temperature is increased in spite of increase in extinction coefficient. In order to find the reason of this fact, ratio of absorption to extinction for various nanospheres in Plasmon frequency is shown in Figure (2).

Figure 2. Variations of absorption to extinction ratio and scattering to extinction ratio for Moscovium nanospheres with various radiuses.

Heat distribution (Figure 3) shows that temperature is uniformly distributed throughout the nanoparticles which are due to high thermal conductivity of Moscovium.

In this section, core–shell structure of Moscovium and silica is chosen. The core of a nanosphere with 45 (nm) radius and silica layer thickness of 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 nanometers are considered. The results show that increase in silica thickness leads to increase in extinction coefficient and shift in Plasmon wavelength of nanoparticles, to some extent.

Figure 3. Maximum increase in temperature for spherical nanoparticles with radius of 45 (nm) at Plasmon wavelength of 685 (nm).

According to Figure (4), silica shell causes to considerable increase in temperature of Moscovium nanoparticles but by more increase in silica thickness, its effects are decreased. Heat distribution (Figure 5) shows that temperature is uniformly distributed throughout metallic core as well as silica shell. However, silica temperature is considerably lower than core temperature due to its lower thermal conductivity. In fact, silica layer prohibits heat transfer from metal to the surrounding aqueous environment due to low thermal conductivity and hence, temperature of nanoparticles has more increase in temperature. Increasing the thickness of silica shell leads to increase in its thermal conductivity and hence, leads to attenuate in increase in nanoparticles temperature.

Figure 4. Maximum increase in temperature for core–shell Moscovium nanospheres with various thicknesses of silica shell.

Figure 5. Maximum increase in temperature for core–shell nanoparticles with radius of 45 (nm) and silica thickness of 10 (nm) at Plasmon wavelength of 701 (nm).
Figure (6) is drawn. This graph shows that variation of nanorod dimension ratio leads to considerable shift in Plasmon wavelength. This fact also allows regulating the Plasmon frequency to place in near IR zone. Light absorption by body tissues is lower in this zone of spectrum and hence, nanorods are more appropriate for optothermal human cancer cells, tissues and tumors treatment methods.

![Fig 6](image)

**Figure 6. Extinction cross section area for Moscovium nanorods with effective radius of 45 (nm) and various dimension ratios.**

Variations of temperature in Moscovium nanorods with two effective radius and various dimension ratios are shown in Figure (7). By increase in length (a) to radius (b) of nanorod, temperature is increased.

![Fig 7](image)

**Figure 7. Maximum increase in temperature for nanorods with effective radius of 20 and 45 (nm) and various dimension ratios.**

4. Conclusion and Summary

The calculations showed that in Moscovium nanoparticles, light absorption in Plasmon frequency causes to increase in temperature of the surrounding environment of nanoparticles. In addition, it showed that adding a thin silica layer around the Moscovium nanospheres increases their temperatures. Calculations of nanorods showed that due to ability for shifting surface Plasmon frequency toward longer wavelength as well as more increase in temperature, this nanostructure is more appropriate for medical applications such as optothermal human cancer cells, tissues and tumors treatments.

5. Acknowledgements

Authors are supported by an American International Standards Institute (AISI) Future Fellowship Grant FT12010093734741. We acknowledge Ms. Isabelle Villena for instrumental support and Dr. Michael N. Cocchi for constructing graphical abstract figures. We gratefully acknowledge Prof. Dr. Christopher Brown for proof reading the manuscript. Synchrotron beam time was awarded by the National Synchrotron Light Source (NSLS–II) under the merit-based proposal scheme.

6. References


61] Li, J.; Liang, J.; Li, L.; Ren, F.; Hu, W.; Li, J.; Qi, S.; Pei, Q. Heatable Capacitive Touch Screen Sensors Based on Transparent Composite Electrodes Comprising Silver Nanowires and a Furan/Maleimide Diels-Alder Cycloaddition Polymer. ACS Nano 2014, 8, 12874–12882, 10.1021/nn506610p


Wang, Q. Study of Perfluorophosphonic Acid Surface Modifications on ZnO Nanoparticles. Materials, 2017, 10, 1–16, 10.3390/ma10121363
Pharmacology, Phytochemistry and Ethnomedicine, Volume 1, Issue 1, Pages 15–19, 2015.


[111] A. Heidari, “Measurement the Amount of Vitamin D2 (Ergocalciferol), Vitamin D3 (Cholecalciferol) and Absorbable Calcium (Ca²⁺), Iron (II) (Fe²⁺), Magnesium (Mg²⁺), Phosphate (PO₄³⁻) and Zinc (Zn²⁺) in Apricot Using High–Performance Liquid Chromatography (HPLC) and Spectroscopic Techniques”, J Biom Biostat 7: 292, 2016.

[112] A. Heidari, “Spectroscopy and Quantum Mechanics of the Helium Dimer (He₂⁺), Neon Dimer (Ne₂⁺), Argon Dimer (Ar₂⁺), Krypton Dimer (Kr₂⁺), Xenon Dimer (Xe₂⁺), Radon Dimer(Rn₂⁺) and Ununoctium Dimer (Uuo₂⁺) Molecular Cations”, Chem Sci J 7: e112, 2016.


[120] A. Heidari, “Discriminate between Antibacterial and Non–Antibacterial Drugs Artificial Neural Networks of a Multilayer Perceptron (MLP) Type Using a Set of Topological Descaptors”, J Heavy Met Toxicity Dis. 1: 2, 2016.


Combined Theoretical and Computational Study”, Transl Biomed. 7: 2, 2016.


[193] A. Heidari, “Pros and Cons Controversy on Molecular Imaging and Dynamics of Double–Standard DNA/RNA of Human Preserving Stem Cells–Binding Nano Molecules with Androgens/Anabolic Steroids (AAS) or Testosterone


[204] A. Heidari, “Vibrational Decihertz (dHz), Centihertz (cHz), Millihertz (mHz), Microhertz (μHz), Nanohertz (nHz), Picohertz (pHz), Femtohertz (fHz), Attohertz (aHz), Zettahertz (ZhZ) and Yoctohertz (yHz) Imaging and Spectroscopy Comparative Study on Malignant and Benign Human Cancer Cells and Tissues under Synchrotron Radiation”, International Journal of Biomedicine, 7 (4), 335–340, 2017.


[214] A. Heidari, “Comparative Study on Malignant and Benign Human Cancer Cells and Tissues with the Passage of


[235] A. Heidari, “Biomedical Instrumentation and Applications of Biospectroscopic Methods and Techniques in Malignant and Benign Human Cancer Cells and Tissues


[258] A. Heidari, “Cadaverine (1,5–Pentanediamine or Pentamethylenediamine), Diethyl Azodicarboxylate (DEAD or DEADCAT) and Putrescine (Tetramethylenediamine) Nano Molecules Incorporation into the Nano Polymeric Matrix (NPM) by Immersion of the Nano Polymeric Modified Electrode (NPME) as Molecular Enzymes and Drug Targets for Human Cancer Cells, Tissues and Tumors Treatment under Synchrotron and Synchrocyclotron Radiations”, Hiv and Sexual Health Open Access Open Journal. 1 (1): 4–11, 2018.


[280] A. Heidari, “Fucitol, Pterodactyladiene, DEAD or DEADCAT (DeEthyl AzoDiCarboxylaTe), Skatole, the NanoPutians, Thebacon, Pikachurin, Tie Fighter, Spermidine and Mirasorvone Nano Molecules Incorporation into the Nano Polymeric Matrix (NPM) by Immersion of the Nano Polymeric Modified Electrode (NPME) as Molecular Enzymes and Drug Targets for Human Cancer Cells, Tissues and Tumors Treatment under Synchrotron and Synchrocyclotron Radiations”, Glob Imaging Insights, Volume 3 (4): 1–8, 2018.


