Magna Scientia Advanced Research and Reviews

eISSN: 2582-9394

Cross Ref DOI: 10.30574/msarr

Journal homepage: https://magnascientiapub.com/journals/msarr/

(RESEARCH ARTICLE)

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Modeling SARS-CoV-2 and preventing COVID-19 pandemic

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Magna Scientia Advanced Research and Reviews, 2022, 06(02), 024–033

Publication history: Received on 17 October 2022; revised on 26 November 2022; accepted on 29 November 2022

Article DOI: https://doi.org/10.30574/msarr.2022.6.2.0077

Abstract

Backgrounds: Since December 2019, COVID-19 pandemic has globally killed more than 6.602 millions, infected more than 635.2 millions of people and lasted almost three years, as of 11/22/2022. The pandemic is still killing more than 7,261 and infecting more than 2.259 millions of people per week in the whole world today. We think the rates of the fatality, infection and the long term of the pandemic are related to proliferation characteristics and biological structures of SARS-CoV-2.

Methods and Objectives: We apply theories of biology, ligand field, biophysics, biochemistry, virology, classic electrodynamics, and published biological data, to model proliferation characteristics and biological structures of SARS-CoV-2.

Modeling Results and Outcomes: We coin a concept: quasi identical biological objects carry the quasi identical biological information (spatial, temporal, electromagnetic and mass properties), and they cannot occupy the same biological envelope if their repulsive forces between them are stronger than the resistances. We propose two models of exclusions. Exclusion of RNA (DNA) strands: No normally and naturally replicated quasi identical RNA (DNA) strands can occupy the same virus. Exclusion of viruses: No normally and naturally proliferated quasi identical viruses can occupy the same biological host cell. For a SARS-CoV-2, we model the charged ssRNA and N proteins as a negatively charged central body, the charged proteins in the biological membrane as dynamic ligands, the electric field between the center and ligands as a dynamic ligand field.

Conclusions: The biological models of exclusions of RNA strands in a virus and viruses in a host cell qualitatively respectively answer the questions why or how there is only one mature ssRNA strand inside a SARS-CoV-2 membrane envelope and the virus proliferate; it is suitable to extend or analogize the ligand field theory to illustrate the stability of SARS-CoV-2 in biophysical structures (topologic constructions). Our models could be applicable to other biological objects.

Keywords: SARS-CoV-2; RNA (DNA); Strand; Exclusions; Dynamic Ligand; Field; Virus; Extension; COVID-19; Electric; Charge; Potential

1. Introduction

Since December 2019, COVID-19 pandemic has globally killed more than 6.602 millions, infected more than 635.2 millions of people and lasted almost three years, as of 11/22/2022. The pandemic is still killing more than 7,261 and infecting more than 2.259 millions of people per week in the whole world today [1].

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Additionally, a SARS-CoV-2 variant has been demonstrated to be associated with increase in detrimental change in COVID-19 epidemiology; or change in clinical disease presentation; or decrease in effectiveness of public health and social measures [2].

Therefore, we think, how to cure (or prevent) COVID-19 is still an urgent issue in clinics and health care fields; the rates of the fatality, infection and long term of the pandemic are related to proliferation characteristics and biological structures (topologic construction) of SARS-CoV-2.

Severe acute respiratory syndrome coronavirus 2 (SARSCoV-2) is a class IV, enveloped, positive-sense and single-stranded RNA (ssRNA) virus that causes the disease COVID-19 [3-4].

SARS-CoV-2 is a beta-coronavirus whose genome is about 30 kb and size is about 100 nm in diameter [5]. The viral RNA is packaged by the structural proteins to assemble viral particles at the ERGICER-Golgi intermediate compartment. The four major structural proteins are the spike (S) surface glycoprotein, the membrane (M) matrix protein, the nucleocapsid (N) protein, and the envelope (E) protein [6].

The RNA is negatively charged [7]. M and N are highly positively charged proteins [8].

The SARS-CoV-2 N protein is a positively charged and may be critical for protein: RNA interaction [3].

The M (glycol) proteins span the membrane bilayer [9-10], bind to all other structural proteins, and promote completion of viral assembly by stabilizing the N protein-RNA complex inside the internal virion [11].

The viral spike (S) protein of coronaviruses facilities the attachment to the cellular receptor [12]. The stalk part is negatively charged, the top part of the spike molecule (S protein), especially the receptor binding domain, remains positively charged [13].

The E protein is the smallest and has the lowest copy number of the membrane proteins [14-15]. The E protein has an even net charge distribution on both sides of the membrane and is translated in the endoplasmic reticulum (ER) and accumulates in the Golgi. Then, the E protein monomer self-assembles into an oligomer that functions as an ion channel [16].

Analyzing data of SARSCoV-2, we notice that there is always only one mature ssRNA is inside SARS-CoV-2 membrane envelop, and we ask ourselves questions: Why or how is there only one mature ssRNA inside SARS-CoV-2 membrane envelop? Do distributions of the virus proteins provide extra forces to facilitate the stabilization of SARS-CoV-2 in biological structures (topologic constructions)?

Ligand field theory describes the bonding and molecular orbital of complex compounds. It represents an application of molecular orbital theory to transition metal complexes. The bonding, orbital and complexes are investigated by means of symmetry concepts. The best features of both the valence-bond picture and the crystal field theory are incorporated in the ligand field theory [17].

The bonding is essentially due to electrostatic interaction between positive central ion and the dipoles or ions of the coordinated groups. The groups attached the central ion are called ligands. These ligands are assumed to behave as point negative charges, and create an electrostatic field around the central ion, which produces an additional bonding effect called the ligand field stabilization energy [18].

Therefore, another question we ask ourselves is, is it suitable to extend or analogize the ligand field theory to illustrate the stability of SARS-CoV-2 in biophysical structures (topologic constructions)?

Based on classical electromagnetism and molecular biology of the cell, we previously defined a memory as stored information that can be remembered and recalled to respond to other memories or information; a biological cell as a memory unit; DNA genes, mRNA, proteins and other cellular molecules (components) as sub-memory units. We also defined three types of sub-cellular memories: the static are stored in genes (sets) in DNA strands, the dynamic are stored in RNA (sets or strands) and the functional are stored in proteins (sets). We think memories include spatial and temporal fields or virtual particles, such as the electric (major), magnetic (minor) and the gravitational (inconsiderable), as well as the structured matters (represented with charges and masses), the electric charges and fields play an important role in the biological information and (or) memories [19].

Using the above definitions of biological information and (or) memories, knowledges of classical electromagnetism and molecular biology of the cell, we proposed our models of natural and normal mitosis (with asters) and cytokinesis, for animal cells in M phase. The models describe the following exclusions.

- Chromosomes Exclusion: No normally and naturally replicated chromosomes can occupy the same nucleus without growing sizes of the biological nucleus and cell [20].
- Nuclei Exclusion: No normally and naturally doubled biological nuclei can occupy the same biological cell if the doubled size of nuclei is not far smaller than size of the biological cell [20].

We think, the replicated or doubled biological objects carry the identical (inherited) information of their parents, the spontaneous, repulsive and strong electric fields and forces play major roles for the exclusions; the principles of our previous models of the above exclusions can be also applied to that for virus proliferation or replication; and the ligand field theory is suitable to extend or analogize to illustrate the stability of biological structure (topologic construction) of a SARS-CoV-2.

However, we have not found any investigation of SARS-CoV-2 with the above exclusion principle and ligand field theory.

Recently, we proposed multiple models to prevent COVID-19 pandemic at a level of human tissues [21-22].

In this paper, based on molecular biology, virology, biophysical and biochemical theory and classic electromagnetism, we propose our models of SARS-CoV-2 at molecular and virus levels: exclusions of RNA strands and viruses, and extension (analogy) of ligand field theory; we also discuss variations of viruses, to understand the virus proliferation, structure and pandemic. We believe our models and discussions will be helpful to prevent COVID-19 pandemic.

2. Methods

In this investigation we apply theories of biology [7], ligand field [17-18], biophysical chemistry [18], classic electrodynamics [23-24], biochemistry [25], virology [26], and published biological data [1-16, 27-29].

3. Results

Based on our previous models of exclusions of biological chromosomes and nuclei in a biological nucleus or cell [20], see introduction of this paper, we coin a concept in this study: quasi identical biological objects carry (have) the quasi identical (almost 100% the same) biological information (spatial, temporal, electromagnetic and mass properties), and they cannot occupy (be in) the same biological envelope (system) if the their repulsive forces between them are stronger than the resistances.

3.1. Exclusions of RNA Strands and Viruses

The forces that drive the assembly of virus particles include hydrophobic and electrostatic interactions. Only rarely are covalent bonds involved in holding together the subunits. In biological terms, this means that protein-protein, protein-nucleic acid, and protein-lipid interactions are involved [26].

In most biomedical applications, the magnetic and gravitational influences are ignored because they are too small compared with that of the electric [19]. Therefore, we focus on the electric interaction in this study.

We consider the RNA, proteins and lipid molecules as (quasi) dielectrics, condensed or paracrystalline state matters; the electric charges of RNA, proteins and lipids produce the electric fields and potentials, cause the electrical space to curve and organize the virus structures, the mechanism is the same or similar to that of a biological cell [20]; the field and potential spaces drive the nucleocapsid proteins and membranes (lipids and proteins) to distribute as close as possible to the RNA cores (spherical viruses with icosahedral capsids [27] and curved equipotential surfaces or spaces. Figure 1 illustrates the spherical coordinate system and Figure 2 shows two sets of ssRNA + Nucleocapsid N proteins in one host biological cell. The ssRNA and Nucleocapsid N proteins are considered as a whole.

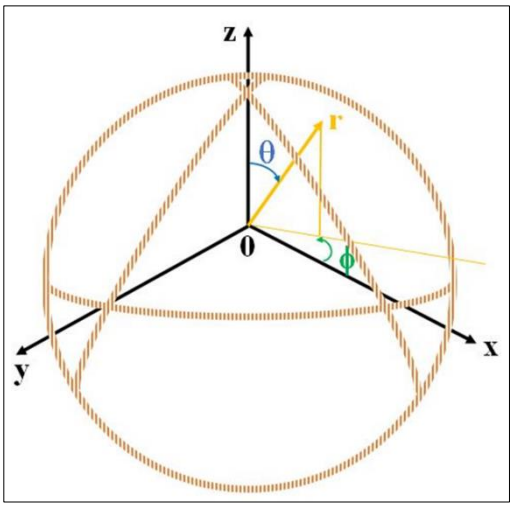

Figure 1 A spherical coordinate system (r, ϵ θ, ϵ ϕ) embedded in a Cartesian coordinate system (x, y, z). See the text. The draw is not to the scale

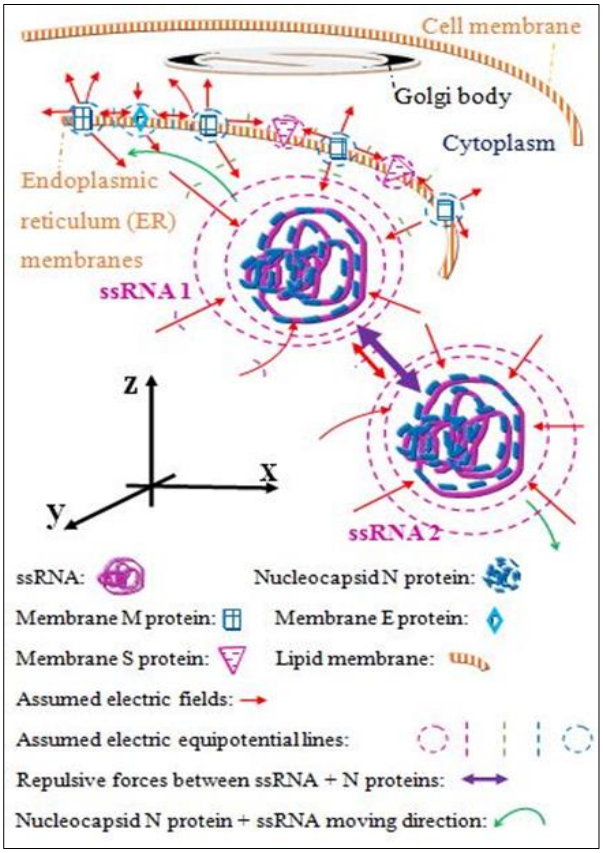

Figure 2 Two sets of ssRNA + Nucleocapsid N proteins in one host biological cell. The ssRNA and Nucleocapsid N proteins are considered as a whole. Red, blue and green colors respectively denote negative, positive and 0 electric charges, potentials and fields. When the moving whole (ssRNA and Nucleocapsid N proteins) are passing the membrane, the membrane bends around the whole roughly conforming the equipotential surfaces by the electric field (red arrows) forces. The figure is in x and z plane (two dimensions). The model is based on published biological data. [5, 8, 9] See the text. The draw is not to the scale

Though SARS-CoV-1 and SARS-CoV-2 are geometrically polyhedral formations [27], we morphologically approximate them as spheres rather than icosahedrons, to simplify our models [28-29, 10, 26].

Viruses invade host cells to replicate themselves by using the host resources, such as (ATP) energy, lipid and amino acids molecules and (or) making machines of RNA (DNA). A SARS-CoV-2 is accomplished with a global biological membrane when it is leaving the host cell [28-29, 10, 26].

In this study, we consider the negatively charged ssRNA and the positively charged nucleoproteins (icosahedral capsids) [4] as a whole; the negative charges of ssRNA are only partially shielded by the positive charges of the nucleocapsid N proteins; therefore the whole has a net negatively charged distribution.

We think the mechanisms of the separation of the replicated RNA strands and the releasing of the replicated viruses out of the host cells are the same as or in a similar way to that described with our previous models of mitosis [20].

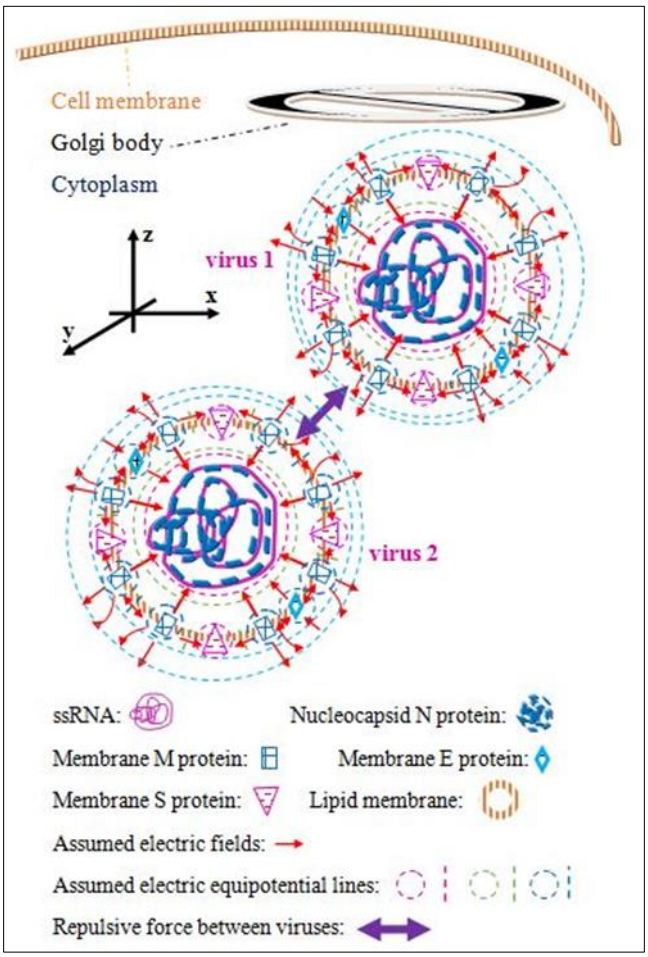

Figure 3 Two (quasi) identical SARS-CoV-2 with complete membranes are in one host biological cell. Red, blue and green colors respectively denote negative, positive and 0 electric charges, potentials and fields. ssRNA and Nucleocapsid N proteins are considered as a whole. The thicker the line, the higher the absolute value. The figure is in x and z plane (two dimensions). The model is based on published biological data. [5, 8, 9] See the text. The draw is not to the scale

Therefore, we model the replicated ssRNA strands and (or) SARS-CoV-2 as quasi identical biological objects, they respectively carry (have) the quasi identical (almost 100% the same) biological information (spatial, temporal, electromagnetic and mass properties). The quasi identical ssRNA strands can not occupy (in the) same virus and the quasi identical viruses can not occupy (be in) the same host biological cell, if their repulsive forces between them are respectively stronger than the correspondent resistances.

The spontaneous, repulsive and strong electric forces separate the ssRNA (and nucleocapsid N proteins) into different viruses (Figure 2) and push the SARS-CoV-2 progenies off from the host cell membrane (exocytosis) (Figure 3).

The more general statements of our exclusion models of RNA (DNA) strands and viruses are as the following:

Exclusion of RNA (DNA) strands: No normally and naturally replicated quasi identical RNA (DNA) strands (biological information carriers) can occupy (be in) the same virus without growing sizes of the envelope, if the repulsive forces are stronger than the resistances; the spontaneous, repulsive and strong electromagnetic field (EMF) forces between (or among) the quasi identical RNA (DNA) strands separate the strands into different virus envelopes. The mechanism is the same as or similar to the exclusion of the chromosomes of eukaryotes [20].

Exclusion of viruses: No normally and naturally proliferated quasi identical viruses (biological information carriers) can occupy (be in) the same biological host cell, if the repulsive forces are stronger than the resistances, i.e., if the virus sizes are not far smaller than the size of the biological host cell, the spontaneous, repulsive and electromagnetic field (EMF) forces between (or among) the quasi identical viruses exclude the viruses out of the host biological cell. The mechanism is the same as or similar to the biological nuclei exclusion of eukaryotes [20].

The above models of exclusions qualitatively answer our questions why or how there is only one mature ssRNA strand inside a SARS-CoV-2 membrane envelope and the virus proliferation.

3.2. Extension (Analogy) of Ligand Field Theory

Figure 4 is an illustration of ligand field theory: complex $[Co(NH_3)_6]^{3+}$, Co^{3+} ion is at the center and 6 NH_3 molecules as ligands are symmetrically around Co^{3+} ion [18]. The central ion and ligand molecules construct a ligand (electric) field, the symmetrical and attract electric field forces produce additional bonding effects to stabilize the complex.

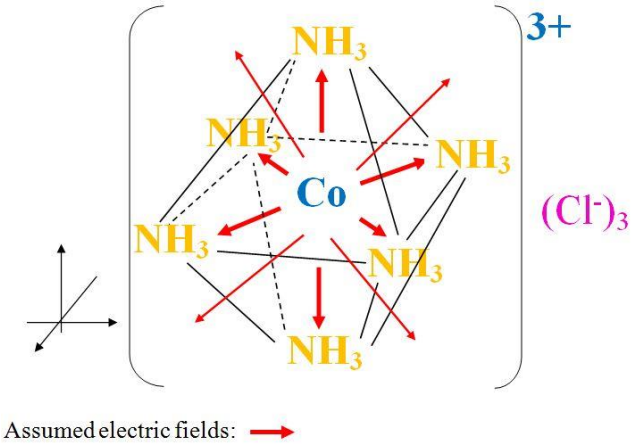

Figure 4 An illustration of ligand field theory: Complex $[Co(NH_3)_6]^{3+}$, Co^{3+} ion is at the center and 6 NH_3 molecules as ligands are around Co^{3+} ion. [18] The compound is $[Co(NH_3)_6]^{3+}(Cl^-)_3$. The figure is in three dimensions. See the text. The draw is not to the scale

Proteins are embedded in this bilayer sheet, held by hydrophobic interactions between the membrane lipids and hydrophobic domains in the proteins. The membrane mosaic is fluid because most of the interactions among its components are noncovalent, leaving individual lipid and protein molecules free to move laterally in the plane of the membrane [25].

We think virus external shapes or forms are mostly determined by their internal macro molecular structures, such as RNA (DNA) strands and proteins. The relationship between the internal and external is similar to that the regular form of crystals is the result of a regular internal arrangement of molecules [18].

For a matured SARS-CoV-2, to simplify our models, we consider the following approximations based on published information [30, 6]: a ssRNA and its N proteins are a spherical whole in spatial structure, the whole have a spherically symmetrical electrical charge distribution about the spherical center; the produced electric fields are centrally oriented, i.e., the fields are central force fields (Figure 5); the replicated N, M, E and S proteins are globally, dynamically and symmetrically arranged about the center by the electric forces.

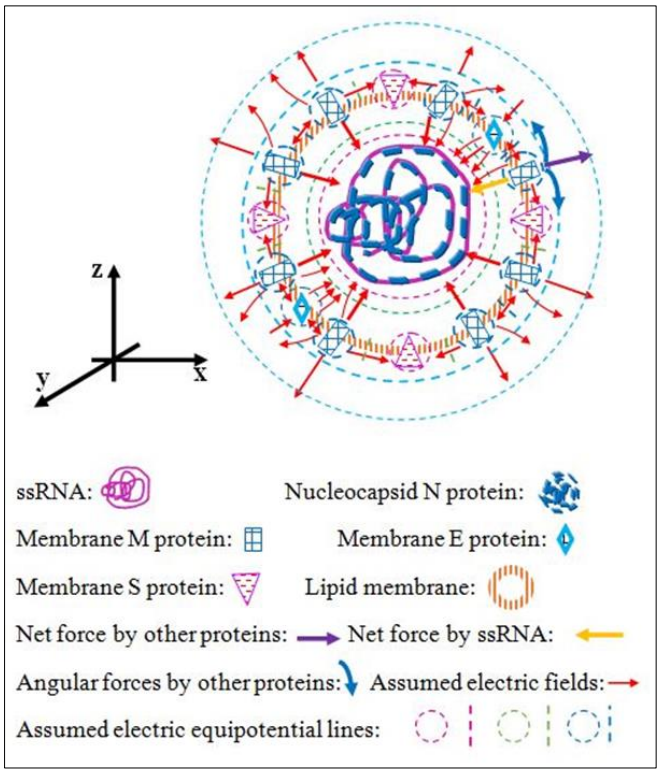

Figure5 A SARS-CoV-2 with a complete membrane in equilibrium or bound states. The ssRNA and Nucleocapsid N proteins are considered as a whole. Red, blue and green colors respectively denote negative, positive and 0 electric charges, potentials and fields. The thicker the lines, the higher the absolute values. The net force by the other proteins is balanced by that of the ssRNA. The figure is in x and z plane (two dimensions). The model is based on published biological data [5, 8, 9]. See Figure 1 and the text. The draw is not to the scale

Based on the above approximations and published information, analogizing ligand field theory [17-18], we model the charged ssRNA and N proteins as a negatively charged central body, the charged proteins in the biological membrane as dynamic ligands (coordinated groups), the electric field between the center and ligands as a dynamic ligand field, and the correspondent energy as a dynamic ligand field energy (Figure 5). We think the ligand and non-ligand fields form a superposition state of the electric fields and the dynamic ligand field energy makes the virus more stable in biophysical structures than that without the ligand.

Our extension model of the ligand field theory indicates: the virus membrane components, (charged) proteins or lipids are approximately symmetric about the virus center (Figures 5); the forces, applied by the other proteins, on each protein, are canceled each other in the angular directions and is balanced by that of the central body (the whole of the ssRNA and Nucleocapsid N proteins) in the radial direction; the central forces are approximately the same in all radial directions and stabilize the global structure (topology) of the virus.

Therefore, we think it is suitable to extend or analogize the ligand field theory to illustrate the stability of SARS-CoV-2 in biophysical structures (topologic constructions).

When the virus constructs its inner structure and surface, its components arrange and move with the principle of variation (minimum energy: The criterion for quality in the variational method is making the ground state energy as low as possible) in the curved equipotential surfaces and in a bound (equilibrium) states; the virus costs the minimum works, therefore its inner energy is at the lowest state. The models in this paper is consistent to that we obtained with electric forces in our previous study [20] and that obtained by minimizing the free energy of membranes under the area and volume (most and approximate sphere or ball) constraints in biological chemistry [25] or thermodynamics [31-32].

4. Discussions

The structure formation of a SARS-CoV-2 can also be explained with thermodynamics, such as surface or interface tensionsm [33] or other theories.

Our extended and dynamic ligand field model describes an interaction of dynamic electric field forces that are quasi symmetric about a center and centrally oriented. The ligand field theory in physical chemistry is involved in chemical bonds or molecular orbitals [18]. Although our extended and dynamic ligand field model is not the same as the ligand field in physical chemistry, our model qualitatively illustrates the structures and movements of SARS-CoV-2 with electrodynamics (electromagnetism) and by an intuitive analogy of the ligand field theory.

We used to classified cellular biological stabilities as inner and external stabilities, and to define the inner stability as inheritance fidelity of DNA genome in divided cells, the external stability as contact inhibition of divided cells. A complete stability means the both inner and external stabilities are satisfied. A biological cellular controllability measure the ability the normal parent cells control the cellular divisions into normal children cells [19].

If we extend the above biological cellular stabilities and controllability to SARS-CoV-2 or other viruses, we believe the biological virus stabilities and controllability are much lower than that of biological cells, i.e., the virus variation rates are much higher than that of biological cells.

Variations of viruses could closely correlate fidelity of the RNA or DNA replications. The replication of almost all viruses has adverse effects on the infected cell, inhibiting cellular synthesis of RNA, DNA or proteins. In general, viral nucleic acid replication is more error-prone than cellular nucleic acid replication [34]. We think: one of the major reasons why or how the viruses dominate the synthesis in the host cells and mutate more easily than (human) cells is that the replications of the virus' RNA (DNA) and protein have lower potential energy barriers or higher affinity than that of the normal host cells [35]. Additionally virus RNA (DNA) synthesis has no or less error-correcting mechanism [7]. Therefore the virus replications have lower fidelities than that of the normal host cells, the mechanism of the low fidelities of virus dominant syntheses could be the same as or similar to that of a tumor or cancer cell.

Although our models in this paper is focused in the study of Class IV: Single-stranded (+) sense RNA, we believe the principles of the models are also applicable to other classes of viruses and other quasi identical biological objects.

Viruses are between living and inanimate objects, they are the simplest (partial) life objects and they have almost all characteristics of a life object except they have to proliferate themselves in a host living cell. Therefore, the investigation of viruses is significant not only to life and non-life sciences but also to the transformation science between the living and inanimate objects.

Any non-side effect (harmless) materials with negative or positive charges or poles, such as C_2H_5-OH (sipping or smelling 1 ml per hour, 60% - 70%) [35], $CH_3)_2$CH-OH (external using only, (70%) [36], could be used to destroy or inhibit the protein spikes of the viruses. We think the inhibition or disinfection of the SARS-CoV-2 (COVID-19) could be because the geometry (symmetries) of the viruses are changed, by the external electrical fields produced by the sanitizers, therefore, the energy states of the proteins, ssRNA strands or viruses are changed.

5. Conclusion

In this study, the biological models of exclusions of RNA strands in a virus and viruses in a host cell qualitatively respectively answer the questions why or how there is only one mature ssRNA strand inside a SARS-CoV-2 membrane envelope and the virus proliferate; it is suitable to extend or analogize the ligand field theory to illustrate the stability of SARS-CoV-2 in biophysical structures (topologic constructions).

Compliance with ethical standards

Acknowledgments

We thank Vivien Cheng for suggestions.

Disclosure of conflict of interest

There is not any conflict of interest between the authors or any persons.

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