

Frontier Orbitals, Combustion and Redox Transfer from a Fermionic-Bosonic Orbital Perspective

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Abstract

Oxygenations are highly exergonic, yet combustion of organic matter is not spontaneous in an atmosphere that is 21% O₂. Electrons are fermions with a quantum spin number s of $1/2\hbar$. An orbital containing a single electron with $s = 1/2$ is fermionic. Orbitals can contain a maximum of two electrons with antiparallel spins, *i.e.*, spin magnetic quantum numbers m_s of $1/2$ and $-1/2$. An orbital filled by an electron couple has $s = 0$ and bosonic character. The multiplicity of a reactant is defined as $|2(S)| + 1$ where S is the total spin quantum number. The Wigner spin conservation rules state that multiplicity is conserved. The transmission coefficient κ of absolute reaction rate theory also indicates the necessity for spin conservation. Burning is fermionic combustion that occurs when sufficient energy is applied to a bosonic molecule to cause homolytic bond cleavage yielding fermionic products capable of reaction with the bifermionic frontier orbitals of triplet multiplicity O₂. Neutrophil leucocytes kill microorganisms by bosonic combustion and employ two mechanisms for changing the multiplicity of O₂ from triplet to singlet. Microorganisms, composed of bosonic singlet multiplicity molecules, do not directly react with bifermionic O₂, but are highly susceptible to electrophilic attack by bosonic electronically excited singlet molecular oxygen (¹O₂^{*}). Hydride ion (H⁻) transfer is the common mode of cytoplasmic redox metabolism. Bosonic transfer of an orbital electron couple protects from damage by obviating fermionic reaction with bifermionic O₂. Bosonic coupled electron transfer raises the consideration that quantum tunneling might be involved in facilitating such redox transfer.

Keywords

Fermion, Boson, Orbital, Spin, Combustion, Redox Transfer, Tunneling

1. Introduction and Background

A wavefunction (ψ) defines a quantum system. An orbital is described by ψ_{n,l,m_l} where n is the principle quantum number, l is the azimuthal or angular momentum quantum number, and m_l is the magnetic quantum number. An electron occupying an orbital is described by the wave function ψ_{n,l,m_l,s,m_s} where the electron-spin quantum number s describes the total spin and the spin magnetic quantum number m_s describes each electron spin as $1/2$ or $-1/2$ [1] [2].

According to the exchange principle, a pair of particles, a and b , can be described by a wavefunction $\psi(a, b)$. Exchanging the particles generates a new wavefunction $\psi(b, a)$. If particles are identical and indistinguishable, their probability distributions will be identical, $\psi^2(a, b) = \psi^2(b, a)$, regardless of the orientation of the particles. When the square roots of the probability distributions yield the wavefunctions $\psi(a, b) = \psi(b, a)$, exchange is symmetric and the particles are bosons. When the wavefunctions $\psi(a, b) = -\psi(b, a)$, exchange is antisymmetric and the particles are fermions. Bosons obey ordinary commutation. Rotating a boson through 360 degrees returns it to its original state, $\psi \xrightarrow{360^\circ} \psi$. Bosons are symmetric particles with integral spin. Photons are bosons with zero mass and integer spin, fermions anti-commute, Rotating a fermion through 360 degrees, $\psi \xrightarrow{360^\circ} -\psi$, changes the sign or phase of the fermion, but does not return the particle to its original state. An additional 360 degrees rotation, $-\psi \xrightarrow{360^\circ} \psi$, is required to return the antisymmetric particle to its original state. Electrons, protons and neutrons are fermions with mass.

Bosons differ from fermions with regard to quantum spin. The natural unit of quantum spin is the reduced Planck's constant (\hbar -bar or \hbar), where $\hbar = h/(2\pi)$. Bosons have spins with integer values. Photons are bosons with a spin value of $1\hbar$. Fermions have spins that are $1/2$ integers. Electrons are fermions with a spin of $1/2\hbar$. Electrons possess intrinsic spin described by the quantum number s . Such spin is independent of orbital motion and is without analogy in classical physics. The spin magnetic quantum number m_s has two spin possibilities: $1/2$ (spin up, \uparrow) or $-1/2$ (spin down, \downarrow). The multiplicity of an atom or molecule equals $|2(S)| + 1$ where S is the total spin.

2. Fermionic and Bosonic Orbitals

Fermions can combine to yield a wavefunction with bosonic character. An alpha particle made up of four fermions is bosonic [3]. An electron is a fermion. As such, an orbital filled by a single electron has an $s = 1/2$ and fermionic character [4] [5]. An orbital filled by an antisymmetric electron couple has $s = 0$ and bosonic character. The frontier orbitals of atoms and molecules are directly involved in reaction chemistry and include the lowest unoccupied (LU(A)MO), the highest occupied (HO(A)MO), and the single electron occupied (SO(A)MO) atomic (A) or molecular (M) orbitals [6].

The vast majority of reactions observed in organic and biochemistry involve singlet multiplicity reactants. Reactions involve frontier LUMO and HOMO are

bosonic. Free radical reactions involve fermionic frontier orbitals, *i.e.*, SO(A)MO. Reaction chemistry can be approached from a fermionic-bosonic orbital perspective.

Consistent with the fermion nature of electrons, Pauli's exclusion principle limits an orbital to a maximum of two antiparallel electrons, *i.e.*, m_s of $1/2$ (\uparrow) and $-1/2$ (\downarrow). In **Figure 1**, note that the lower energy 1s and 2s orbitals of atomic N each contain two antiparallel electrons, *i.e.*, an orbital couple with $s = 0$. These orbitals are closed to reaction chemistry. The frontier orbitals of atomic N include the three 2p orbitals. These 2p orbitals are degenerate, *i.e.*, each orbital has the same energy. Each 2p orbital contains a single fermionic electron. Hund's maximum multiplicity rule states that the electrons in degenerate singly occupied orbitals will have parallel spins [7]. As such, each of the three 2p frontier orbitals of N have an $s = 1/2$ and the S of N is $3(1/2)$. The spin multiplicity, *i.e.*, $|2(S)| + 1$, for N is thus $|2(3/2)| + 1 = 4$. Stated differently, atomic nitrogen is a tri-radical with quartet spin multiplicity. Each 2P orbital of N is a SOAO, and as such, atomic N is trifermonic. As depicted in **Figure 1** and stated in **Table 1**, the product of reacting two quartet multiplicity N atoms is singlet multiplicity N_2 .

The lower energy 1s and 2s orbitals of N all contain coupled antiparallel electrons with $s = 0$. These non-frontier bosonic orbitals do not participate in reaction. Likewise, the sigma bonding (σ) and antibonding (σ^*) orbitals of N_2 , derived from the 1s and 2s orbitals of the atomic N's, are bosonic and closed to reaction chemistry. The frontier π bonding orbitals of N_2 are both filled by an electron couple with $s = 0$ and have bosonic character. In its ground state, N_2 is singlet multiplicity, triple bonded and bosonic.

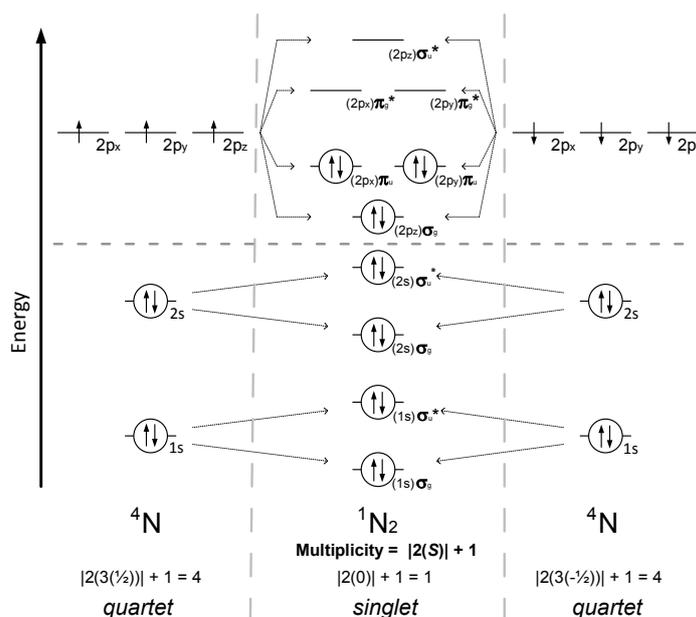


Figure 1. Orbital diagrams for atomic nitrogen (N), shown on left and right sides of the figure and separated by dashed vertical lines. The resulting molecular orbital diagram for N_2 is shown in the center. The filled σ_g and π_u bonding orbitals, shown above the dashed horizontal line, are responsible for the triple bond of N_2 .

Table 1. Conservation of spin multiplicity from a fermionic-bosonic orbital perspective.

Reactant A	Reactant B	Reaction Complex
Singlet bosonic	Singlet bosonic	Singlet bosonic
Singlet bosonic	Doublet fermionic	Doublet fermionic
Singlet bosonic	Triplet bifermionic	Triplet bifermionic
Singlet bosonic	Quartet trifermonic	Quartet trifermonic
Doublet fermionic	Doublet fermionic	Singlet bosonic
Doublet fermionic	Triplet bifermionic	Doublet fermionic
Doublet fermionic	Quartet trifermonic	Triplet bifermionic
Triplet bifermionic	Triplet bifermionic	Singlet bosonic
Triplet bifermionic	Quartet trifermonic	Doublet fermionic
Quartet trifermonic	Quartet trifermonic	Singlet bosonic

3. Spin Conservation

3.1. Transmission Coefficient of Absolute Reaction Rate Theory

Absolute reaction rate theory states that the rate of a chemical reaction requires that reactants first combine to form an activated complex,

$$k = \kappa(kT/h)K^*$$

where k is the rate, κ is the transmission coefficient, kT/h has the dimensions of frequency and K^* is the equilibrium constant for the activated complex. The transmission coefficient, κ , for typical reactions approximates unity, *i.e.*, each activated complex yields product, but not every activated complex at the potential-energy barrier will cross over to product [8]. The value of κ decreases by several orders of magnitude in reactions involving change in spin state [8].

3.2. Wigner Spin Conservation from a Fermionic-Bosonic Perspective

The Wigner spin conservation rules state that a reacting system resists any change in spin angular momentum, *i.e.*, multiplicity [9] [10]. The total spin number, S , of an atom or molecule defines its multiplicity; *i.e.*, $|2S| + 1 = \text{multiplicity}$. When $S = 0$, the multiplicity is singlet, when $S = 1/2$, the multiplicity is doublet, when $S = 1/2 + 1/2$, the multiplicity is triplet, et cetera. Reactions involving change in multiplicity have transmission coefficient, κ , values of less than 10^{-4} . The spin states or multiplicities of the reactants determine the spin state or multiplicity of the activated complex, and are conserved in the spin states or multiplicities of the resulting product or products. For example, if the impossibility of orbital overlap is ignored and reaction is assumed to involve a bosonic singlet multiplicity molecule and a bifermionic triplet multiplicity molecule, then the activated complex must have a bifermionic triplet multiplicity, and bifermionic triplet multiplicity must be conserved in the product or products. These and other possibilities are described in **Table 1**.

With regard to multiplicity, singlet-singlet reactions are allowed and yield singlet products. From a frontier orbital perspective, bosonic HOMO-LUMO interactions are allowed and yield bosonic products. For example, reaction of singlet multiplicity hypochlorite (OCl^-) with singlet multiplicity hydrogen peroxide (H_2O_2) yields singlet multiplicity water (H_2O), singlet multiplicity chloride (Cl^-) and electronically excited singlet multiplicity molecular oxygen ($^1\text{O}_2^*$). Singlet multiplicity reactants produce singlet multiplicity products. Spin conservation requires $^1\text{O}_2^*$, not triplet multiplicity $^3\text{O}_2$, as the product of the $\text{H}_2\text{O}_2\text{-OCl}^-$ reaction. Production of $^1\text{O}_2^*$ is required for spin conservation, but violates Hund's maximum multiplicity rule [11], and as such, $^1\text{O}_2^*$ is electronically excited with a lifetime of about a microsecond [12]. As illustrated in **Figure 2**, $^1\text{O}_2^*$ relaxes to its triplet ground state by emitting a near infrared photon [13].

Bosonic frontier orbital interactions make up the vast majority of organic and biochemical reaction. Reactions involving a singlet with either a doublet, triplet or quartet multiplicity molecule must conserve spin. If bosonic-fermionic reaction occurs, the reaction product will retain the multiplicity of the fermionic reactant. Relative to frontier orbital considerations, such reactions require highly improbable LUMO-SOMO interaction. However, reactions involving doublet-doublet, triplet-triplet and quartet-quartet multiplicity reactants all yield singlet multiplicity products. Based on frontier orbital considerations, these fermion-fermion, bifermion-bifermion, and trifermission-trifermission reactions involve SOMO-SOMO interactions and produce bosonic products. The unfavourability of singlet-triplet, *i.e.*, bosonic-bifermionic, reaction is well illustrated by considering the reaction of ground state triplet multiplicity ($S = 1/2 + 1/2$ or $-1/2 + -1/2$) molecular oxygen ($^3\text{O}_2$) with a singlet multiplicity ($S = 0$) substrate molecule.

As illustrated in **Figure 2**, $^3\text{O}_2$ has two singly occupied frontier orbitals. As defined by Hund's maximum multiplicity rule, the lowest energy or ground state of $^3\text{O}_2$ is achieved when both of its pi antibonding (π_g^*) frontier orbitals have one electron, *i.e.*, each π_g^* orbital has the same m_s , *i.e.*, $1/2 + 1/2$ or $-1/2 + -1/2$ [11]. Since the two frontier orbitals of $^3\text{O}_2$ are both fermionic, $^3\text{O}_2$ is described as bifermionic. Oxygen is the second most electronegative element, and as such, organic oxygenation reactions are highly exergonic, but frontier orbital interaction are highly improbable, and combustion is not spontaneous.

Radicals react with radicals. Frontier orbital interactions involving SOMO-SOMO reactants are easily conceived. The products of such doublet-doublet reactions are singlet. In SOMO-SOMO reaction, the fermionic electrons of each SOMO couple to produce a bosonic product. For example, frontier orbital interaction of the fermionic π_g^* SOMO of doublet multiplicity hydroperoxyl radical ($^2\text{HO}_2$) with the fermionic π_g^* SOMO orbital of doublet multiplicity superoxide radical ($^2\text{O}_2^-$) yields singlet multiplicity hydrogen peroxide (H_2O_2) and electronically excited singlet multiplicity molecular oxygen ($^1\text{O}_2^*$) [14].

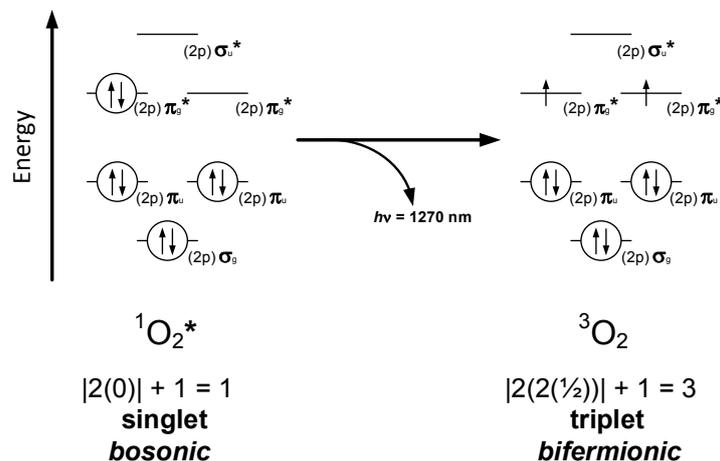


Figure 2. The frontier orbitals of electronically excited ${}^1\text{O}_2^*$ violate Hund's maximum multiplicity rule (left) and has a microsecond life time relaxing to ground state ${}^3\text{O}_2$ (right) by near-infrared photon (1270 nm) emission.

The role of ${}^3\text{O}_2$ in quenching the phosphorescence from relaxation of electronically excited triplet multiplicity dye (${}^3\text{dye}^*$) is explained by triplet-triplet annihilation yielding bosonic products. This same triplet-triplet quenching is responsible for photodynamic action. Reaction of the electronically excited triplet dye (${}^3\text{dye}^*$) with ${}^3\text{O}_2$ returns the dye to its ground state (${}^1\text{dye}$) and photodynamically generates ${}^1\text{O}_2^*$ [15] [16].

4. Combustion

Combustion, defined as an act or instance of burning, requires fuel and molecular oxygen, and produces heat and light. The organic molecules that serve as fuel are of singlet multiplicity and present bosonic frontier orbitals that are unreactive with the bifermionic frontier orbitals of ${}^3\text{O}_2$. Consistent with absolute reaction rate theory and the spin conservation rules, such reactions are not spontaneous.

4.1. Fermionic Combustion

To initiate burning, a sufficient amount of energy, e.g., a flame, must be applied to cause homolytic bond cleavage of the singlet multiplicity fuel molecule. Each homolytic cleavage yields two doublet multiplicity SOMO products. These fermionic products can directly react with the bifermionic frontier orbitals of ${}^3\text{O}_2$. Radicals react with radicals. As described in **Table 1**, reaction of a doublet multiplicity (*i.e.*, $S = 1/2$) radical with triplet multiplicity (*i.e.*, $S = -1/2 + -1/2$) molecular oxygen yields doublet multiplicity ($S = -1/2$) product, heat and light. In turn, the doublet multiplicity ($S = -1/2$) product can now react with another triplet multiplicity ($S = 1/2 + 1/2$) ${}^3\text{O}_2$, et cetera, resulting in reaction propagation, *i.e.*, burning. Note that fermionic-fermionic reaction yields bosonic product, and that fermionic-multifermionic reaction yields the least fermionic prod-

uct.

4.2. Bosonic Combustion

The neutrophil leukocyte, a phagocytic white blood cell, is tasked with defending the host animal against a vast variety of pathogenic microorganisms [17]. Fifty years ago, I pondered the possibility that phagocytic leukocytes kill microbes by changing the multiplicity of molecular oxygen from triplet to singlet [18]. From a frontier orbital perspective, changing bifermionic $^3\text{O}_2$ to bosonic $^1\text{O}_2^*$ opens the possibilities for bosonic electrophilic reaction with the bosonic molecular composition of microbes, *i.e.*, bosonic combustion. Conventional fermionic combustions involve highly exergonic oxygenation reactions that generate electronically excited carbonyls that relax by emitting photons in the visible spectrum. The bosonic combustions of neutrophil leukocyte microbicidal action also involve highly exergonic oxygenations that generate electronically excited carbonyls with relaxation by photon emission. Light is emitted when neutrophil leukocytes phagocytose and kill opsonized microbes, and the photon emission or chemiluminescence is proportional to $^3\text{O}_2$ consumption and to glucose metabolism via the hexose monophosphate metabolic (HMP) shunt. As described in the section below, neutrophil leukocytes employ two mechanisms for the conversion of bifermionic $^3\text{O}_2$ to bosonic $^1\text{O}_2^*$. The first involves fermionic-fermionic annihilation, and the second involves myeloperoxidase-mediated bosonic-bosonic reaction.

4.3. Neutrophil Combustive Microbicidal Metabolism

Neutrophil reduced nicotinamide adenine dinucleotide phosphate (NADPH) oxidase controls HMP metabolism by accepting two reducing equivalents from NADPH thus liberating the oxidized NADP^+ that is required for glucose-6-phosphate (G-6-P) dehydrogenase metabolism of glucose. Biochemical dehydrogenations involve hydride (H^-) transfer. The bosonic character of such redox exchange will be considered subsequently. The riboflavin prosthetic group of NADPH oxidase facilitates decoupling of the bosonic electron pair. Riboflavin mediated separation allows fermionic expression of the separated electrons and results in reactive electron capture by bifermionic $^3\text{O}_2$ [14]. The product of such univalent reduction is the doublet multiplicity hydroperoxyl radical ($^2\text{HO}_2$). $^2\text{HO}_2$ is an acid with a pKa of 4.8 that dissociates yielding a proton (H^+) and doublet multiplicity superoxide radical ($^2\text{O}_2^-$). The reaction of fermionic $^2\text{HO}_2$ and fermionic $^2\text{O}_2^-$ is a radical-radical annihilation yielding bosonic singlet multiplicity hydrogen peroxide ($^1\text{H}_2\text{O}_2$) and bosonic electronically excited singlet multiplicity molecular oxygen ($^1\text{O}_2^*$) [19]. As described in **Table 1**, reactions of fermions yield bosonic products.

Neutrophils contain abundant myeloperoxidase (MPO). The haloperoxidase action of MPO provides an additional mechanism for generation of bosonic $^1\text{O}_2^*$. MPO consumes the H_2O_2 and acid (H^+) products of NADPH oxidase ac-

tivity to oxidize chloride (Cl^-) to hypochlorous acid (HOCl) or its conjugate base hypochlorite (OCl^-). All of the reactants and products of MPO haloperoxidase action are singlet multiplicity and present bosonic frontier orbitals. The HOCl/OCl^- produced can further react non-enzymatically with additional H_2O_2 producing Cl^- and $^1\text{O}_2^*$ [20]. MPO can catalyze classical peroxidase activity involving radicals, but such activity is distinct from the acid haloperoxidase action involved in microbicidal action [17].

Generation of $^1\text{O}_2^*$ violates Hund's maximum multiplicity rule; *i.e.*, the electronic configuration with highest multiplicity has the lowest energy. The greater the number of wave functions possible for a system, the lower the energy. Higher multiplicity states produce greater nuclear-electron attraction and are of lower energy [11]. As such, $^1\text{O}_2^*$ is metastable with a lifetime of about a microsecond. This lifetime restricts its potent electrophilic reactivity to within a radius of about 0.2 microns (μm) [12]. Upon phagocytosis, the microbe becomes the locus of neutrophil microbe killing. Generation of the bosonic reactant $^1\text{O}_2^*$ within the phagolysosome space of the neutrophil directly focuses its potent electrophilic reactivity to the target microbe and minimizes collateral damage. Purified MPO selectively binds all gram-negative bacteria tested and can bind and inactivate endotoxin even in the absence of haloperoxidase function [21]. Selective MPO binding to microbes correlates with selective MPO-mediated microbicidal action. Bosonic combustion is limited by the lifetime of $^1\text{O}_2^*$. Such reactive restrictions have the advantage of selectively focusing and confining combustive action to the microbe while avoiding bystander injury to host cells [22].

5. Bosonic Transfer of Reducing Equivalents

Cytoplasmic redox transfers, *i.e.*, pre-cytochrome electron transfers, typically involve the movement of two reducing equivalents from one singlet multiplicity molecule to another, and is described as H^- transfer. Such hydride transfer involves the movement of a proton plus an orbital couple of antiparallel electrons. The orbital couple has a $s = 0$, and as such, transfer is singlet multiplicity and bosonic.

Biological systems are exposed to an atmosphere with abundant O_2 . The bosonic character of biochemical systems provides protection against direct reaction with bifermionic O_2 . As previously considered, any biologic transfer involving a single fermionic electron would open the possibility for direct fermionic reaction with O_2 . The resulting fermionic-bifermionic reaction would produce a fermionic product and the possibility for further fermionic-bifermionic propagation.

Redox transfer of a bosonic orbital electron couple might offer additional advantage. The bosonic nature of the alpha particle facilitates quantum tunneling from the nucleus [23]. The bosonic nature of a Cooper pair of electrons facilitates superconductivity [24]. Alpha particle radiation and Cooper pairing in superconductivity are very different from each other, and both phenomena are very different from biochemical redox electron transfer. However, the commo-

nality of bosonic pairing in quantum tunneling raises suppositions with regard to a possible role in facilitating biological redox transfer.

6. Summary and Conclusion

Reaction chemistry involves frontier orbital interactions. An orbital is fermionic if occupied by a single electron, and bosonic if occupied by an electron pair. With regard to orbital reactivity, bosonic orbitals react with bosonic orbitals generating bosonic products, fermionic orbitals react with fermionic orbitals generating bosonic products, and fermionic orbitals react with bifermionic molecules generating less fermionic products. Fermionic-bosonic reactions are improbable, but the products of any such reaction must conserve the fermionic character of the reaction complex. As a general observation, all reactions favor bosonic products. Burning or fermionic combustion is initiated by homolytic bond cleavage producing fermionic products that react with bifermionic triplet O_2 . The bosonic combustion of neutrophil leukocytes is initiated by changing the multiplicity of O_2 from triplet to singlet allowing bosonic electrophilic dioxygenation. With the exception of cytochrome chain transfer, intermolecular redox reactions involve transfer of an orbital electron pair and are bosonic. Such transfer obviates the possibility for fermionic reaction with bifermionic O_2 and additional fermionic propagation. As a supposition, quantum tunneling might facilitate intermolecular redox transfer of a bosonic orbital electron couple.

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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