

## FROM CORTICAL MICROCOLUMNS TO BRAIN BARCODES

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### ABSTRACT

Artificial neural systems and nervous graph theoretical analysis rely upon the standpoint that the neural code is endowed in logic circuits, *e.g.*, spatio-temporal sequences of ON/OFF spiking neurons. However, this assumption does not fully explain complex brain functions. Here we show how nervous activity, other than logic circuits, could instead depend on topological transformations and symmetry constraints occurring at the micro-level of the cortical microcolumn, *e.g.*, the basic embryological, anatomical and functional unit of the brain. Tubular microcolumns can be flattened in guise of a fullerene-like two-dimensional lattices, equipped with about 80 nodes standing for pyramidal neurons, where neural computations take place. We show how the countless possible combinations of activated neurons embedded in the lattice resemble a barcode. Every different assembly of firing neurons might stand for diverse neural codes, each one responsible for single mental activities. A two-dimensional fullerene-like lattice not just simulates the real microcolumn's microcircuitry, but also allows us to build an artificial network model that, because grounded just on simple topological changes corresponding to pyramidal neuronal activation, is equipped with robustness, plasticity and fastness.

Current computational brain models, based on neural networks performing logic operations (Izhikevich, 2010; Sporns 2013; Ursino et al., 2014), are not able to fully elucidate a large repertoire of brain functions and mental faculties, such as attention and perception, emotions and cognition, memory and learning, higher cognitive processes (decision making, goal-directed choice, etc.) (Gazzaniga, 2009), mind wandering (Andrews-Hanna et al., 2014) and so on. In order to build a versatile network able to simulate the brain function at micro-levels of observation, we introduce a cortical model borrowed from fullerene's geometry, *e.g.*, a method able to evaluate symmetry constraints and topological indices for micro-structures (Koorepazan-Moftakhar et al., 2015). Although its primary application concerns the description of carbon-networks in chemical compounds, this method provides a mathematical treatment that can be used in order to rank topological invariants in the description of neural networks. In particular, the method might apply to description of microcolumns, *e.g.*, the fairly uniform, stereotyped, vertical column-like architecture believed to be the basic embryological/anatomical module and the fundamental processing unit of cortical arrangement (Mountcastle 1997; Jones, 2000). Minicolumns are characterized by modular connectivity with invariant properties that resembles fullerene structures. Indeed, minicolumns display a translational symmetry across their central axis and

rotational symmetry, *i.e.*, displacement in different planes of section. Furthermore, microcolumns are equipped both with transitive symmetry involving geometric scaling of morphometric relations in different cortical areas, and with temporal symmetry involving morphometric relations during cortical maturation (Opris and Casanova, 2014). Because architectonic relations among minicolumnar elements (e.g., pyramidal cells) are conserved under spatial and temporal variations (Casanova et al., 2011), we are allowed to assess the tubular structure of a microcolumn in terms of a 3D cylinder with the typical regular structure of the Fullerene, e.g., a mesh of variously fused hexagons and pentagons. When the cylindrical structure is flattened into a 2D rectangular sheet, we achieve a lattice that allows us to investigate microcolumns' microcircuitry and its operations in a way different from the classical logic of ON/OFF neural firing. Indeed, a Fullerene-like 2D sheet is a structure where countless transformations, dictated by accurate rules and constraints, might occur. They can be compared to a barcode, or a biological matrix, in which every sequence of neuronal activation stands for a mental activity. We may also think to the bronze cup-shaped bells of a carillon, in which every sequence of diverse punchers gives rise to different melodies. In sum, we achieve a fullerene-like brain which activity is dictated by topological transformations taking place just on hexagons and pentagons. Such an approach not only allows us to build a model that faithfully simulates the biological brain activity, but also allows us to assess neural computations in terms of topological relationships and transformations among spiking neurons, instead of parallel or series circuits of logic gates. We also discuss the advantages of such an approach in terms of network fastness, robustness and plasticity.

## MATERIALS AND METHODS

Here we show how microcolumns microcircuitry can be described in terms of fullerene 2D lattices, equipped with the same asymptotic topological behaviour. Fullerenes are 3-connected cubic planar graphs consisting of pentagons and hexagons (Schwerdtfeger et al., 2013). Geometrically, a fullerene is a closed trivalent polyhedral network in which

atoms are arranged in 12 pentagonal and  $\left(\frac{1}{2}n - 10\right)$  hexagonal rings (Fowler et al., 1993; Fowler et al., 2001; Chuang

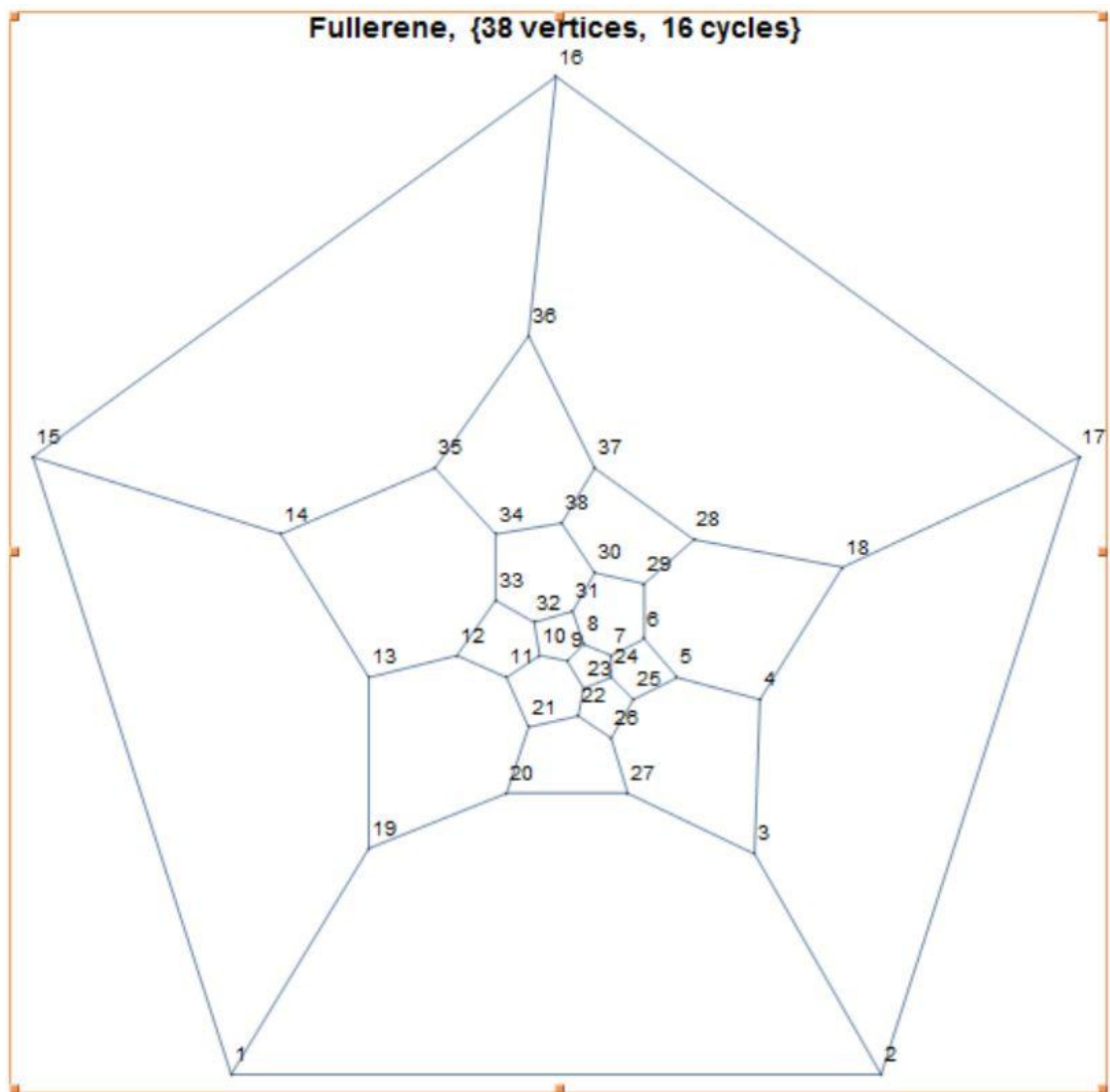
et al., 2009). A regular 2D fullerene is a 3-regular cubic planar graph  $F$  that is generally describable as a mesh of (exactly) 12 variously fused pentagons, and surrounded by distorted graphenic fragments. A sample fullerene is shown in **Figure 1**.

A cortical microcolumn comprises about 80–120 neurons, except in the primary visual cortex where the number doubles. About 80% of such cells are pyramidal neurons. This basic unit circuit forms a series of repeated items across the horizontal extent of the cortex, independent of cortical areal specializations (Jones, 2000): in humans, the transverse diameter of each of the  $2 \times 10^7$ – $2 \times 10^8$  microcolumns is about 28–50  $\mu\text{m}$  (Sporns et al., 2005; Johansson and Lansner, 2007). We can therefore build a biologically-plausible, fullerene-like lattice describing a microcolumn. See **Figures 2A** and **2B** for further details concerning the steps from tubular cortical microcolumns to fullerene-like two-dimensional sheets. In sum, we achieve a 30 microns-width lattice equipped with hexagonal or pentagonal tiling and about 80 nodes (or vertices). Such nodes, standing for the about eighty microcortical pyramidal neurons, are linked by edges (or bonds), e.g., dendritic or axonal connections.

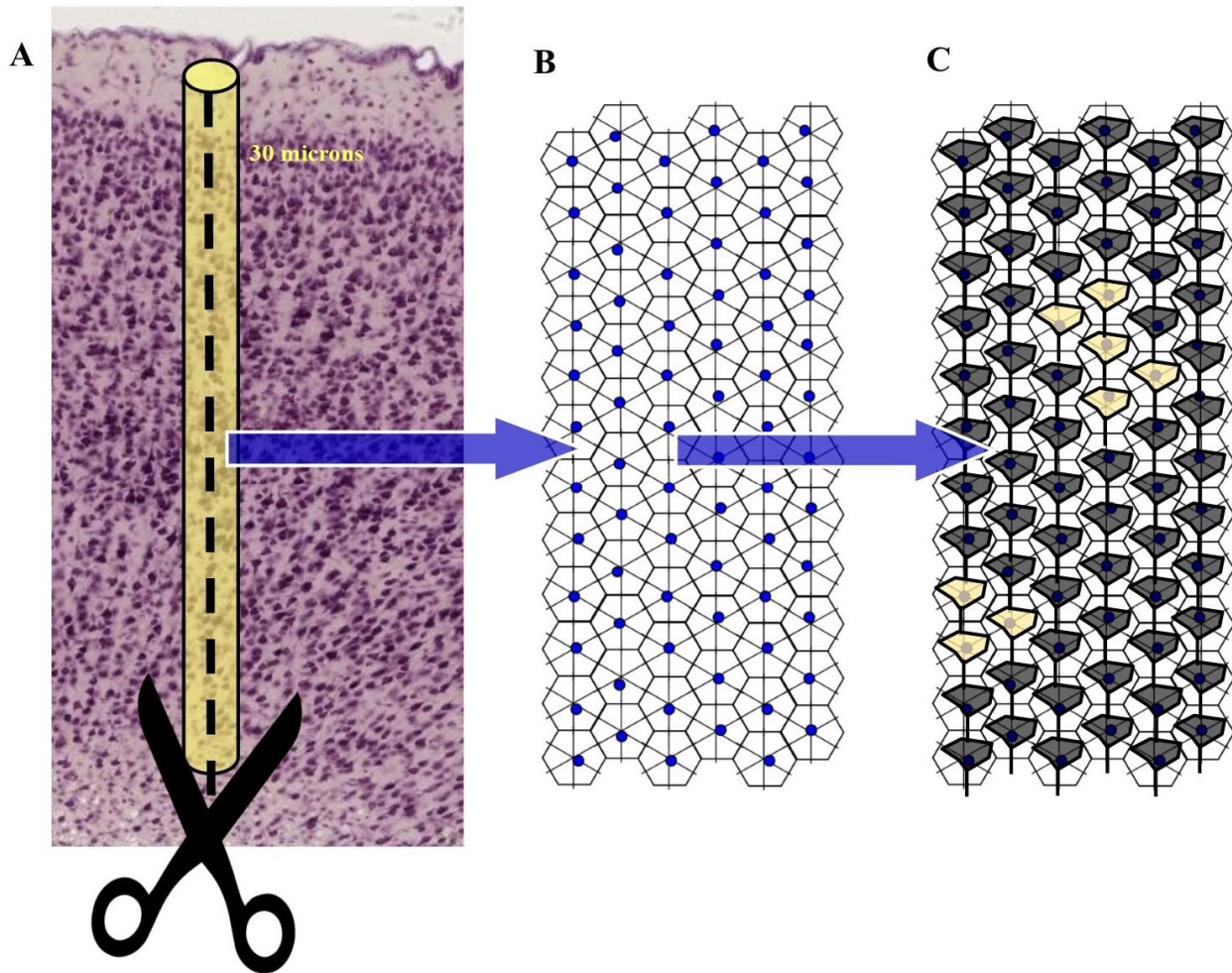
Topological permutations occurring on the hexagonal or pentagonal surface of a fullerene-like lattice can be assessed and calculated. Indeed, methods based on vertex insertions or deletions and isomerisations on lattices have proven to be very useful, because they allow the formal derivation of one fullerene graph from another (Ori et al., 2014). In particular, the so-called Stone-Wales (SW) transformations produce a rotated figure, without changes in the external connectivity of the fullerene and in the molecular topology outside the represented region of the lattice surface (Babic et al., 1995). In sum, the SW mechanism makes a dipole dislocation extending in the fullerene mesh as a wave.

We hypothesize that such SW transformations might have a counterpart in the real biological activity of microcolumnar microcircuitry. In the nervous case, instead of SW flips on a fullerene surface, we could take into account the changes in firing activation of the about 80 neurons embedded in the nodes. In the case of microcolumns, “permutation” means which pyramidal neurons are sequentially activated and which are deactivated. In other words, SW permutations may be regarded as a set of simple pyramidal neurons which fire simultaneously (**Figure 2C**). Every group of neural “permutations” might stand for a sort of barcode, corresponding to a peculiar mental activity.

Concerning the mathematical apparatus related to symmetries and transformations on nanostructures, see Koorepazan-Moftakhar et al (2015). The Authors assessed the symmetry properties of the automorphism group of the graph, providing the upper limit, fully rooted in topology, on the nanostructure's geometrical symmetry. They also reported the theorems and algorithms which allow a fast computation of topological indices for complex graphs, starting from their structural building elements.



**Figure 1.** Sample fullerene with 38 vertices and 16 cycles. See text for further details.



**Figure 2.** General description of a fullerene-like cortical microcolumn. In **Figure 2A**, the anatomical/functional basic structure of the brain, e.g., the tiny cortical microcolumn, is shaped in guise of a three-dimensional tubular armchair. If we cut the column through an edge, we achieve a flattened two-dimensional fullerene-like grid with exagonal tiling (**Figure 2B**). In the hypothetical case of **Figure 2B**, provided just as an example, the molecular graph stands for a 2D zig-zag lattice, e.g., a flat, open visualization, made of 72 nodes with 6-bonds each. **Figure 2C** depicts a few possible topological transformations that might take place on this flattened microcolumn. Every node is filled with a pyramidal neuron which can be activated (yellow shapes) or deactivated (black shapes). Every set of activated/deactivated neurons gives rise to a different microcolumnar barcode, each one standing for a single mental activity among the countless possible.

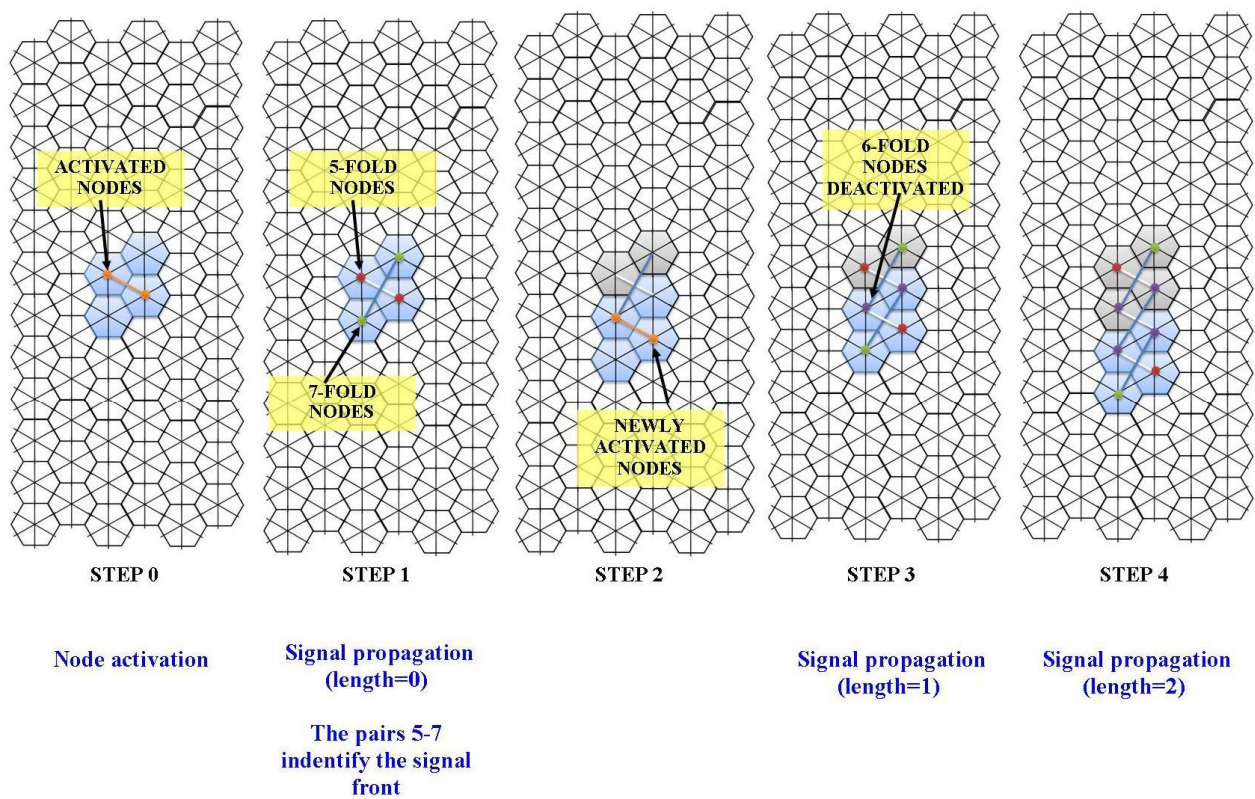
## RESULTS

Here we provide some simulations that show how, starting from a fullerene structure, it is possible to reversibly generate many alternative isomers with a lower structural symmetry, just by twisting two exagons around a central bond (**Figures 3 and 4A**). The possible combinations of permutations (and therefore of simultaneously activated neurons in a fullerene-like microcolumn) are countless: in a lattice of 80 nodes and 2 activities (ON/OFF), we achieve the noteworthy number of  $2^{80}$  possible permutations. Many operations, not shown in Figures, can be performed: edges sharing, interchanging the positions of two hexagons, rotation of a *single* edge, and so on. Because the switches are fully reversible, the edges can be rearranged in countless ways.

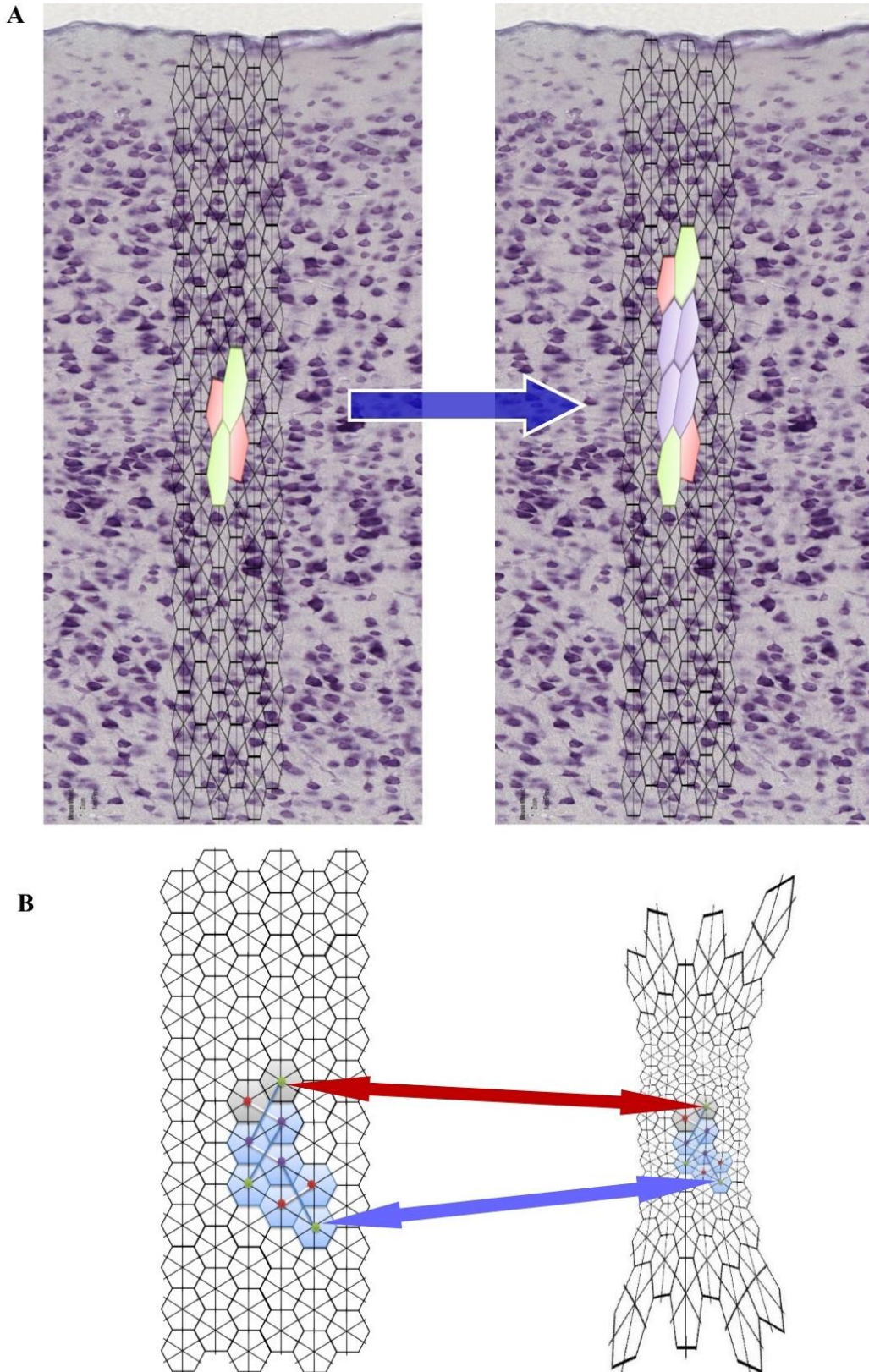
It might be objected that we do not know, due to our current lack of knowledge, whether the microcortical assembly of pyramidal neurons exhibits the proper fullerene-like stereotyped conformation. For example, in our simulation in **Figure 4A**, the lattice exagons appear to be “stretched”. The Borsuk-Ulam theorem (BUT), from algebraic topology, gives us a clue to solve this problem. The original formulation of BUT describes antipodal points with matching



description on spatial manifolds in every dimension, provided the n-sphere is a convex structure with positive curvature (i.e, a ball). However, BUT can be generalized to symmetries occurring either on flat manifolds, or on Riemannian hyperbolic manifolds of constant sectional curvature -1 and concave shape (i.e, a saddle) (Mitroi-Symeonidis, 2015; Tozzi and Peters, 2016). In other words, whether the system components are equipped with concave, convex or flat conformation, it does not matter: we may always find the points with matching description predicted by BUT (Tozzi, 2016). This means that, even if the pyramidal neurons are not arranged into the microcolumn in guise of a perfect fullerene-like structure, we can always describe their activations in terms of transformations on two-dimensional zig-zag lattices (**Figure 4B**).



**Figure 3.** Simulation of a few possible transformations taking place on a flat hexagonal lattice equipped with 72 nodes, 6-bonds each. The lattice stands for the cortical microcolumn containing 72 pyramidal neurons described in **Figure 2C**. Starting from the totally inactive state of 6-fold nodes on 6x12 lattice (displayed in **Figure 2B**), some nodes get activated (**STEP 0**). We may select whatever pair in the mesh. To make an example, after a visual input from the external environment, a few microcolumnar pyramidal neurons start to fire. **STEP1** displays two 5/7 pairs, activated by just rotating the orange bond of **STEP 0**. Signal propagation gives rise to a sequential activation of novel front nodes (**STEP2**), so that the activation wave propagates steps further (**STEPS 3 and 4**). Note that the purple balls, which identify hexagonal nodes deactivated after the passage of the wave, are ready for a possible reversible annihilation of the topological signal.



**Figure 4A.** Topological simulation of propagating signals on a fullerene-like grid embedded in situ into a cortical microcolumn. The stained exagons, depicting SW transformations in lattice's nodes, stand in this case for activated pyramidal neurons. See main text for further details. **Figure 4B:** every kind of transformation in a fullerene molecule leaves the relationships among the single elements unchanged, do to the Borsuk-Ulam theorem's dictates. The Figure shows how a deformation of the original fullerene-like lattice leaves the location of firing neurons unchanged.

## DISCUSSION

We achieved a 2D fullerene-like lattice reproducing microcolumn's microcircuitry. The question now is: given the countless nervous computational models (Van den Heuvel and Sporns, 2011; Friston, 2010; Sengupta et al., 2016), what does a fullerene-like brain theory bring into play, in the evaluation of brain activity? Although our lattice looks like a classical neural network at very first sight, nevertheless it is faster, less energy-consuming, more plastic and stabler. It is also easy to parametrize, because information can be extracted from just a few parametrizing factors. e.g., the simple topological operations taking place on our network. While other approaches emphasize macro-phenotype dynamics, our framework is grounded on dynamics occurring at nervous micro-levels. We assume that the simultaneous firing of different neurons and specific activation sequences might give rise to different topological conformations, each one corresponding to a mental activity (perception, emotion, mind-wandering, calculation, and so on). The brain functional activity is not based on logic nodes as it occurs in conventional networks, but on topological transformations, e.g., functional changes in the position of firing neurons on a barcode.

Our model explains countless mental operations starting just from a relatively simple, stereotyped, highly preserved biological structure, such as the microcolumn. Fullerene-like models, involving any pair of connected nodes (Maruyama and Yamaguchi, 1998), unveil a very rich phenomenology, due to the almost infinite SW rotations that may take place on the corresponding lattice. This allows a countless set of moves, merely dictated by applying SW rotations on its bonds. Unbounded sets correspond to the infinite series of mental operations taking place in our brain. During the synthesis and growth process of a  $C_n$  fullerene, the isomers with isolated pentagons often undergo SW interconversion. If we use a given  $C_n$  isomer as a seed, we may perform a series of moves that give us the capability to build complete sets of fullerene isomers, by simple binding topological bridges (Babic et al., 1994). Therefore, both isomerization maps and complete isomer space's description can be achieved from a single known conformation. In the same guise, the primal embryonal microcolumn is able to give rise to countless combinations in microcircuitry in the mature individual. Indeed, starting from the single vertical template of about 80 pyramidal neurons that colonizes the whole cortex during embryonal life, countless barcodes might be built with time passing. In touch with catalysts that promote fullerene transformations able to stabilize its transition states, we hypothesize that the habituation to repeated stimuli during the first years of life could give rise to more stable and permanent transformations of the microcolumn's barcode.

Fullerene-like networks are fast, because they use simple transformations. Starting from each randomly built string of  $C_n$  fullerene, one may directly generate a certain number of new isomers using just SW flips, instead of immediately searching for a new one. It improves computational speed, because the number of steps required by every operation is reduced. A simple increase in the order of the SW transformations allows us to connect more microcolumns: this means that dual structures, given by the combination of many microcolumns, can be easily built by joining the reciprocal space. In the same way as the tuning of the nanoparticle/substrate interaction provides unique ways of controlling the nanotube synthesis, fullerene-like, microcolumnar neural networks might provide the fine-grain functional barcode's modularity required by different brain functions (Gomez-Ballesteros et al., 2015). It means that modifications in reciprocal connectivity among adjacent microcolumns allow a larger repertoire of barcode configurations and, therefore, of mental operations.

Fullerene-like networks take time to become efficient, because SW transformations are less favoured by an energetic point of view. Therefore, the building of novel barcodes is a slow, time-consuming process. By a biological point of view, this is in touch with the slow development of mental operations' competence in young Primates (Skeide and Friederici, 2016). Vice versa, a fullerene-like biological neural network gives to adult Primates unvaluable advantages in terms of energy sparing. Incorporation of pentagons, occurring at an early stage of nucleation pathway for single-wall nanotubes, leads to a very efficient system, because the number of dangling bonds is reduced and changes towards more entropic curvatures are achieved (Fan et al., 2003). To make an example, fullerenes produced by the overlap of 12 nanocones which no direct pentagon fusion display very high thermodynamic stability, steady topological configurations and minimized graph invariants (Vukicevic et al., 2011; Ori et al., 2014). In mental terms, a fullerene-like microcolumnar structure is associated with minimal wiring costs and fast synchronization/information transfer (Stam and Reijneveld, 2007). In touch with neural networks derived from the principle of minimum frustration for protein folding (Tozzi et al., 2016), the fullerene-like approach points towards a perception/decision apparatus constrained towards very low energetic levels, but just in long timescales, in order that prediction signals are conveyed by the sole long-standing past experiences.

In sum, we make available a novel approach that allows us to evaluate brain activity in terms of topological and graph theoretical properties of fullerenes. This is a very fertile field of research: current efforts focus on the unsolved mathematical problems concerning fullerenes, e.g., how to generate all possible non-isomorphic graphs for a fixed vertex count, or to calculate the number of distinct Hamiltonian cycles. Researchers are developing 2D graphs and 3D structures for many different fullerenes, ranging from  $N=20$  to 20,000 vertices, in order to evaluate various different graph-theoretical algorithms (Schwerdtfeger et al., 2015). Such powerful tools could be, in a near future, applied to



the assessment of neural networks, in order to achieve a double task: improving our understanding of biological brain function in situ, and building more powerful artificial machines able to simulate cortical activities. Our framework also provides a link with human neurologic and psychiatric diseases. Experimental data and molecular dynamic simulations suggest that defects during the nucleation and growth of graphene alter the physical/chemical properties of carbon nanostructures (Hashimoto et al., 2004), strongly deteriorating their functional state. An increase in energetic constraints, as it occurs, for example, during ageing or central nervous system's diseases, makes it easy to generate defects in the fullerene-like lattice, with subsequent decrease in system's free-energy and functional integrity. Our theoretical framework, cast in a biologically informed fashion, has the potential to be operationalized and assessed empirically. Indeed, the presence of a microcolumnar barcode predicted by a fullerene-like brain will be easily testable, once more powerful high density neurotechniques will be available, capable of capturing the simultaneous activity of large populations of microcolumnar pyramidal neurons, (Koster et al., 2014). To make an example, if we could be able to evaluate the specific microcolumnar pyramidal neurons which fire during every mental activity (e.g., visual tasks, emotions, and so on) in order to achieve a fullerene-like structure filled with the corresponding activated nodes, we could attain a series of different grids or matrices, each one standing for a mental function. We suggest to analyze primate temporal cortex or other associations cortices, instead of the widely studied rodents' barrel cortex or the primates' visual cortex, because the former display a notable sterotypy (Jones, 2000), which may prove to be a better model.

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