# Hidden geometry of human connectomes: a key to higher-order brain functional differences

With its complex circuits, the brain enables the entire human activity, psychology, and behaviour. Its evolutionary adaptation evolved towards a complex structure that supports its functional features. Studies have shown that information processing relies on mechanisms of self-organized criticality (self-regulated bursting dynamics with long-range temporal correlations) supported by the specific organization of brain connections. Hence, quantifying the brain functional structure holds excellent prospects for understanding brain dynamics, psychology, pathology, and cognition.

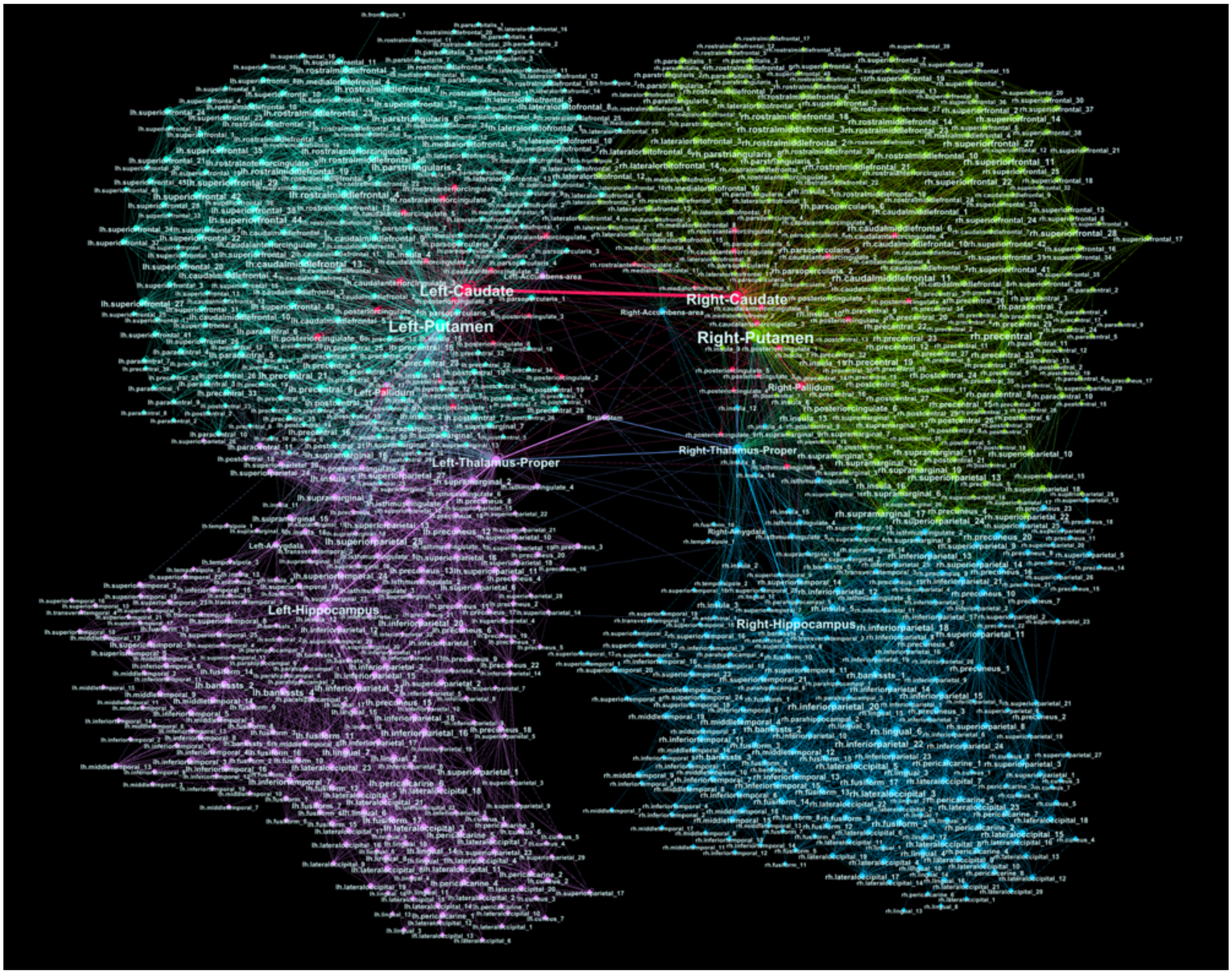


Fig. 1. Consensus Female Connectome consisting of the edges common to 100 healthy individuals is generated by applying the brain mapping tools at the Budapest reference connectome server (https://pitgroup.org/connectome/) based on the diffusion imaging data from Human Connectome Project. Nodes are 1015 anatomical brain regions, indicated by the labels, while 11339 edges are white-matter connections established by one million fibres tracked; colours indicate different mesoscopic-scale communities — the image by BT, using Gephi (https://gephi.org/) graph visualization.

Mathematical modelling of the brain involves a range of algorithms that help interpret the imaging data. Diffusion tensor imaging data have been readily mapped onto the structural brain network (connectome). The network nodes are anatomical grey-matter regions interconnected via white-matter fibre bundles, cf. Figure 1. In recent years, network mapping opened up a new research avenue of brain structure-function interdependences, using advanced graph theory and algebraic topology methods. Our study extends the standard network's theory beyond pairwise connections to determine patterns of higher-order structures. They are geometrically described as triangles, tetrahedrons and higher cliques involving different brain regions. At a larger scale, these simplicial complexes are arranged into five functionally different brain segments, corresponding to the network's communities, as shown in Figure 1. Deciphering how these geometrical descriptors of all sizes are mutually interconnected reveals the entire hierarchical organisation of human connectomes.

Knowing the complete architecture of the human connectome helps elucidate some fundamental features of the brain's functional geometry. Specifically, the graph is 3/2-hyperbolic with short paths, enabling efficient transmissions of information between distant brain areas. The topology hubs (nodes with the most significant connectivity and weights of edges, and the number of simplexes of all orders attached to them) appear to be eight central brain regions (Putamen, Caudate, Hippocampus and Thalamus-Proper in the left and right cerebral hemispheres), making a "rich-club structure". The identified core network around these hubs represents the part of the human connectome through which the hubs connect distinct parts of the brain via simplexes of different sizes. Moreover, beyond the mere number of edges, the structure of simplicial complexes of female and male connectomes unveils the essential sex-related differences. Notably, the female consensus connectome appears better connected in all topology measures than the corresponding male connectome. Potentially, the structural differences between the connectomes in specific neurological disorders (vs. healthy individuals) can be identified using these topological measures. Finally, the precise architecture of simplicial complexes in the human connectome provides a basis for realistic modelling towards the emergent brain dynamics with the higher-order interactions embedded in the underlying geometry.

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## Publication

Functional Geometry of Human Connectomes

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# ADVANCED MODELLING AND DESIGN OF LEAD-FREE PIEZOCOMPOSITES

*The effects of coupling, nonlocality, and nonlinearities*

## Significance

Noteworthy literature has shown that composite lead-free piezoelectric ceramic exhibits excellent piezoelectric properties. In addition to this, lead-free piezocomposites offer the promise of an environmentally-friendly alternative to lead-based materials for conversion of mechanical stimuli into electrical energy. As such, they have drawn worldwide attention in academia and research. Nonetheless, lead-free materials lag behind lead-based materials in terms of their performance. The performance issues can be typically addressed by tuning the mechanical electrical, and crystalline structural properties of the matrix and the piezoelectric inclusions. In fact, various design pathways have been proposed. More so, noteworthy efforts to both model and experimentally demonstrate these design pathways have also been reported. However, in the aspect of design, most of these efforts overlook the contributions due to several important physical effects.

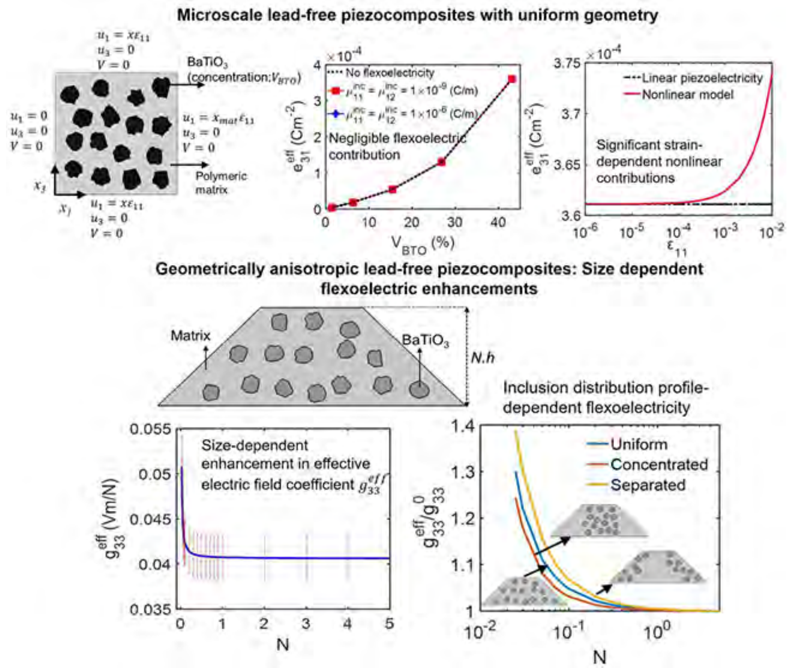
Generally, lead-free piezocomposites are an ecofriendly route for sensing and harvesting energy from mechanical stimuli and it is important to develop accurate models which can capture essential physical processes underlying their performance. Unfortunately, current piezocomposite design heavily relies on the linear piezoelectric model which neglect nonlocal and nonlinear electro-elastic processes. To address this, Dr. Jagdish A. Krishnaswamy (Post-doctoral fellow) and Professor Roderick Melnik from the Wilfrid Laurier University in Canada, in collaboration with Dr. Federico C. Buroni, Dr. Luis Rodriguez-Tembleque and Professor Andres Saez at the University of Sevilla in Spain developed a new and more accurate modelling paradigm to determine the contributions from nonlocal flexoelectric and nonlinear electrostrictive effects towards the performance of lead-free piezocomposites. Their work is currently published in the research journal, *Composite Structures*.

In their approach, the research team first developed a fully coupled electro-elastic model, starting from free-energy considerations, which could simultaneously account for the linear-piezoelectric, nonlinear and nonlocal effects in a lead-free composite architecture. Next, they evaluated the contributions of each of these effects towards the electro-elastic response of a two-component piezocomposite consisting of a polymer matrix with embedded piezoelectric micro-sized inclusions. Overall, they evaluated the contribution of the effects in a three-component composite architecture consisting of a CNT-modified matrix with polycrystalline piezoelectric inclusions.

The authors reported that in the case of microscale randomly shaped piezoelectric inclusions which represent a practical scenario, the flexoelectric effect did not contribute appreciably towards the piezoelectric response. However, the nonlinear electrostrictive effects imparted significant strain-dependent responses. Further, in nano-modified composites, the team found out that the nonlinear electro-mechanical coupling can have different effects on the transverse and the longitudinal electro-elastic responses. In particular, the longitudinal electric field response, with the nonlinear contribution, was seen to be less sensitive to the polycrystalline structure of the piezoelectric inclusions.

As an important extension of this effort, the group recently applied the developed model to understand size-dependent flexoelectricity in geometrically anisotropic piezocomposite structures. Taking an example of a two-dimensional tapered structure, the group was able to demonstrate significant size-dependent enhancements in the piezoelectric response at small length scales. The best enhancements were observed at lower inclusion concentrations and with the inclusions positioned along the tapered surfaces rather than in the bulk of the composite. This serves as a demonstration that significantly high piezoelectric responses can be obtained at low inclusion concentrations by strategically tuning the shape of the composite structure and the size and spatial distribution of the inclusions.

In summary, the study developed a mathematical paradigm to model piezoelectric composites by taking into account important physical effects such as nonlocal flexoelectric and nonlinear electro-strictive effects. Generally, the observation reported provide critical insight into the nonlinear behavior of piezocomposites and emphasize the importance of developing advanced models to describe electro-elastic behavior. A further significant outcome led to obtaining insights into tuning the shape and size of the composite structure and the piezoelectric inclusions to maximize flexoelectric size-dependent enhancements at low inclusion concentrations to design superior piezoelectric materials. In a statement to *Advances in Engineering*, Dr. Jagdish A. Krishnaswamy, first author emphasized that their models can in fact act as a starting point for the design of efficient piezocomposites and directed experimental efforts to tap into these coupled electromechanical effects to improve piezoelectric performance.

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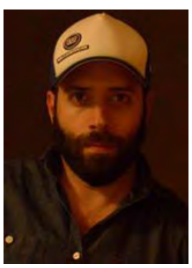
**Roderick Melnik** is a Full Professor at the Wilfrid Laurier University in Waterloo, Canada. He is a Tier I Canada Research Chair in Mathematical Modelling. He is affiliated also with the University of Waterloo as well as with the BCAM Research Center in Europe. Before joining Laurier, Professor Melnik held senior professorial and research positions in the USA, Europe, and Australia. He remains associated with Syddansk University in Denmark where he served as Head of Mathematical Modelling and Engineering Mathematics at the Mads Clausen Institute for a number of years. Later, he was a Full Professor in the Computational Analysis and 2 Modelling Program at the Louisiana Tech University in the USA from where he moved to Canada in 2004. Dr Melnik has also experience in working as a scientist outside of academia. In the late 1990s, he held the position of senior mathematician at the Commonwealth Scientific and Industrial Research Organisation in Sydney, Australia, working in the Division of Mathematical and Information Sciences until he joined the Syddansk University in Denmark as full professor. Dr Melnik received his M.Sc. degree in Applied Mathematics and Ph.D. degree in Computational Mathematics from the Kiev State University in 1985 and 1989, respectively. Since 1989 Professor Melnik held

academic tenures in Europe, Australia, and North America and has published extensively in the field of applied mathematics, computational sciences, and mathematical modelling in sciences and technology. As an active researcher and academic, he is involved in numerous editorial duties and professional services in the applied mathematics, modelling, and a larger scientific community. He is an active member in major professional societies, including the American Society of Mechanical Engineers, Society of Industrial and Applied Mathematics, Canadian Applied and Industrial Mathematics Society and its analogue in Australia ( ANZIAM ), and the New York Academy of Sciences.

Dr Melnik was the recipient of the Hans Christian Andersen Academy Fellowship Award in Denmark with only two such awards that were given annually to researchers worldwide. He was also a visiting fellow at the Isaac Newton Institute of the University of Cambridge in England, at the Institute for Mathematics and its Applications of the University of Minnesota in the USA, the Center of Excellence in Applied Mathematics in Spain, and other research institutions in Europe, North America, and Australia.



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**Dr. Federico C. Buroni** is an Associate Professor in the Department of Mechanical Engineering & Manufacturing at the University of Seville (Spain). He has completed a Mechanical Engineering (5-years) degree from the Universidad Nacional de Mar del Plata in Argentina, and a M.Sc. (2-years) degree from the Universidade Federal do Rio Grande do Sul in Brazil. In 2012 he did his Ph.D thesis entitled “Three-dimensional Green’s functions for anisotropic and multifield materials” at University of Seville, obtaining (highest) “cum laude” designation. His thesis led him to receive the distinction of receiving the “Premio Extraordinario de Doctorado” award. After that he got a position as an Assistant Professor at the University of Seville. During his postdoctoral stage he had the opportunity to complete research 3 stays at the Rutgers University (USA), Universidad Nacional de Mar del Plata (Argentina), and the University of Bristol (UK) as Research Fellow. He has also been awarded with a Postdoctoral

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His scientific contributions have mainly focused on characterizing the dynamic behavior of structures and on applications related to structural integrity. His seminal contributions focused on the development of models and numerical tools (based on the Boundary Element Method and, to a lesser extent, on the Extended Finite Element Method) for the simulation of damage in structural components built with advanced materials. The analyzed material models encompass from composites to functional materials, which present a multi-field coupling between their elastic and electric/magnetic properties (for instance piezoelectric or magnetoelectroelastic materials). More recently, his research has extended to the field of experimental identification of the dynamic properties of structures, with application to aeronautical and, fundamentally, civil engineering structures (monitoring of structural integrity, rehabilitation of masonry constructions, behavior of pedestrian footbridges); as well as to the design and development of sensors based on carbon nanotube-reinforced elements (CNT) and lead-free piezoelectrics, aimed at their subsequent use in damage detection applications.

He has co-authored more than 250 publications, including research papers in scientific journals, books, book chapters and conference proceedings and he has lead several research projects on damage mechanics and structural integrity.

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His research is focused on the design and development of novel multifunctional systems by addressing key challenges relating to material design, functional electronic device design, and system design. On the fundamental front, his contributions pertain to understanding the structure-property relations in materials and functional electronic devices with complex nanoscale and multiscale structures, development of facile fabrication methods for complex structured materials. The particular focus of this aspect of his work in optoelectronic and electromechanical materials and devices.

Another facet of his research includes design and development of sensing systems for self-powered optoelectronic sensing where his contributions center around development of new sensing techniques, smart sensing algorithms, and energy harvesting for ubiquitous sensing. The specific area of interest here is the design and development of self-powered sensing strategies for the internet of things (IoT) in the context of environmental, industrial, and structural monitoring.

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