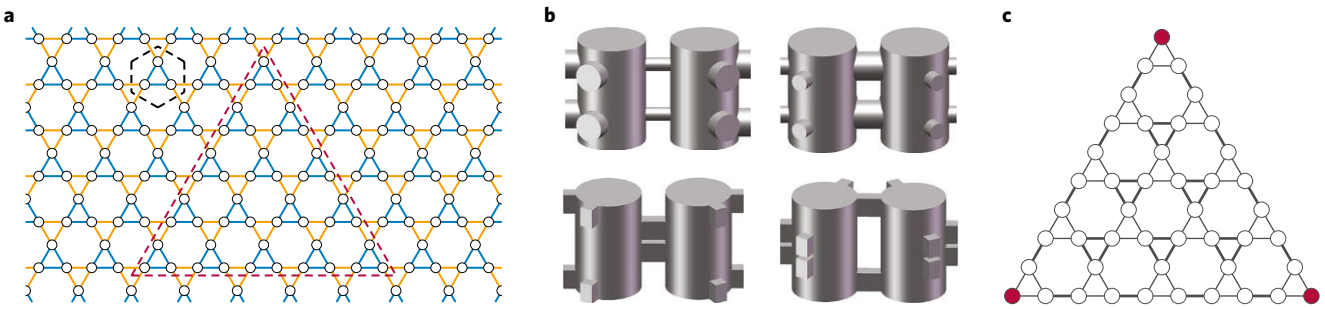


Fig. 1 | Second-order topological acoustic metamaterials on a kagome lattice. a, Kagome lattice with black dashed hexagon marking a unit cell. Empty circles denote 'atoms' that are connected by blue and orange 'bonds'. **b**, 'Atoms' (cylinders) and 'bonds' (tube pairs) designed by Zhang and colleagues[8] (upper panels) and Alù and colleagues[9] (bottom panels). Left panels show blue bonds and right panels show orange bonds. **c**, Three degenerate topological corner states, red coloured, at three corners of the triangular kagome metamaterial, cut along the red dashed lines in **a**.

separation (Fig. 1b, bottom panels). Because the dipole mode in the cylinder has its node on the middle plane of the cylinder (parallel to the flat bottom or top), the orange bond is also stronger than the blue one in this design.

Both teams demonstrate that corner states appear at the corners of the triangular lattice (Fig. 1c), derived by cutting along the red dashed triangle in Fig. 1a, and are robust against the disorders introduced. These findings prove that such constructed 2D acoustic kagome lattices are the second-order topological metamaterials, which can be characterized by the bulk polarizations or the Wannier centres (the topological invariants of the bulk)[5,8,9].

It is interesting that the corner states can only exist at the 60° corners, but not at the 120° corners, if the kagome lattice is cut into a parallelogram shape, as noted by the Zhang team. What is more, the Alù team found that the topological corner states, in addition to the isolated ones, can also be embedded in the continuum of bulk states, which can be excited selectively and separately from the bulk states because of their weak coupling with the bulk states at the corners.

With respect to earlier works with second-order topological metamaterials based on square lattices[6,7], there is an obvious discrepancy in the interpretation. Following previous work[5], both teams believe that the quantized non-zero bulk polarization (or Wannier centre) accounts for the 0D corner states. However, previous works attributed the corner states to the quantized non-zero quadrupole moments in the bulk, while the bulk polarization, on the contrary, vanishes. This discrepancy still remains an open question. Nevertheless, Zhang's and Alù's teams' works represent a marked progress towards a more effective confinement of sound by acoustic metamaterials, which have the potential for several applications, such as local acoustic field enhancement, acoustic trapping and manipulation of particles, and acoustic sensing or probing.

A natural extension of the two teams' works is to further realize higher-order topological metamaterials in 3D, for sound or elastic waves as well as for light or electromagnetic waves. In three dimensions, not only can we expect corner states at the 0D corners in third-order topological metamaterials, but we can also expect for second-order topological metamaterials to host hinge states along the 1D hinges. In addition, because to date the corner states have only been predicted or realized in square and trigonal lattices (2D), and in cubic and tetrahedral lattices (3D), it is instructive to figure out whether corner states can exist in other lattice types, such as corners sharper than the corner of a regular triangle or tetrahedron, which would offer more flexibility for applications. ❐

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2D MATERIALS

Realistic cataloguing of nanopores

Despite an enormous number of nanopores that could, in principle, be formed in atomically thin materials, advanced modelling reveals that in typical experiments rather limited ensembles of most likely nanopores should be observed.

Petr Král

A decade ago, the idea of a graphene nanopore was introduced as an ultimate inorganic material that is able to selectively and rapidly pass atomic and molecular species to a high degree, in analogy to natural protein-based nanopores[1]. Such nanopores were soon prepared in graphene, hBN monolayers and other atomically thin synthetic materials

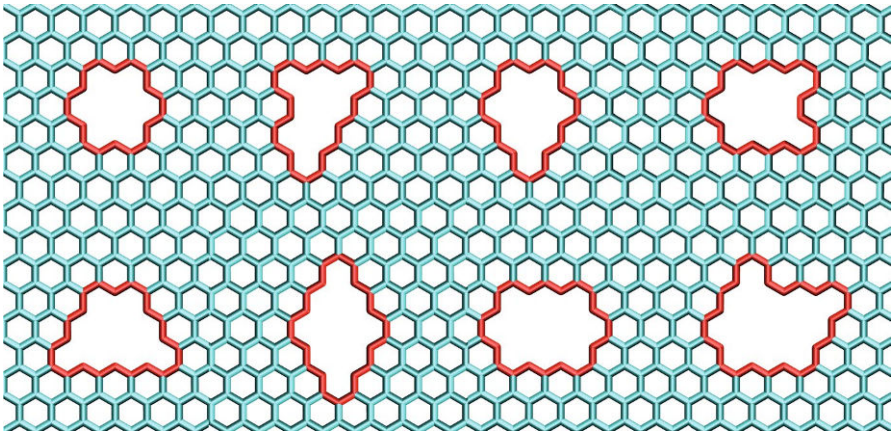


Fig. 1 | Examples of nanopores formed in graphene, as observed in both computational and experimental studies. The number of C atoms removed from graphene to make these nanopore isomers (left to right, top to bottom) is: 6, 6, 7, 8, 8, 8, 10, 12.

with the goal of exploiting separation of atoms and molecules in gas[2] and liquid phases[3], water desalination[4], DNA sequencing[5], efficient energy storage in supercapacitors and batteries[6], and many other attractive applications. However, despite large efforts in the preparation of such nanopores by different methods, precise understanding of the nanopore formation mechanisms and control over the resulting nanopore structures are needed. The lack of detailed knowledge about the nanopores formed makes it difficult to compare various experimental studies performed in such nanoporous materials with appropriate modelling results, and to accomplish intended technological goals. Now, writing in *Nature Materials*, Ananth Govind Rajan and colleagues[7] combine state-of-the-art computational methods to catalogue nanopores that are the most likely to be formed during typical etching experiments in atomically thin materials. The developed hybrid computational approach was implemented in graphene and hBN monolayers, with predictions compared with available experimental observations. It was revealed that the formation of nanopores is kinetically restricted, and the ensembles of the most common nanopores are relatively limited. The knowledge of such ensembles of nanopores should help to establish the basis for correlating theoretical investigations of various phenomena present in these materials with the experimental reality, thus allowing proper design and practical realization of numerous important applications.

Although computational approaches were used in the past to address the problem of nanopore formation in thin layered materials by different techniques, the obtained results had limited agreement with experiments, due to the implemented modelling methods being not fully realistic. In this work, the developed hybrid modelling approach was used to perform computer-based 'experiments' searching for nanopores formed by typical etching methods in atomically thin materials. Govind Rajan and colleagues combined quantum electronic structure methods, kinetic Monte Carlo simulations with thermally controlled and impurity-assisted etching coefficients, and mathematical graphs to catalogue the most-probable structures (isomers) of nanopores formed for given numbers of missing atoms in the vacancy. The graphene nanopore isomers that were the most likely to be observed in these simulations (Fig. 1) had a significant overlap with those experimentally prepared in different laboratories. Moreover, upon conducting a free-energy analysis, it turned out that those nanopore isomers were not the most thermodynamically stable ones, contrary to intuitive expectations, but carried signs of their history of preparation (kinetic pathways). This innovative computational approach could be directly expanded to other nanoporous layered materials, as illustrated by the authors on nanoporous hBN monolayers, where triangular nanopores predicted by the method to be the most common ones were indeed what observed in experiments.

The knowledge of the most likely nanopores to be present in experimental systems could be directly implemented in their practical applications. For example, from the known types of nanopores and the likelihood of their presence in separation membranes, the passage rates of different molecules of fluids through these membranes can be evaluated by molecular dynamics simulations and quantitatively compared with the existing experiments. In a similar way, the knowledge of realistic ensembles of nanopores could be used in evaluation of optical properties of atomically thin materials with known densities and types of nanopores. Overall, while a complete cataloguing and characterizing of nanopores in layered materials might be important from the point of general knowledge, describing the ensembles of the most probable nanopore isomers should reflect well on the existing reality. However, we should keep in mind that when nanopore degradation exists in these materials, the ensembles might require modifications with time.

Historically, we are just at the beginning of a long pathway towards the preparation and understanding of layered synthetic materials possessing nanopores with fully controllable characteristics. Following this

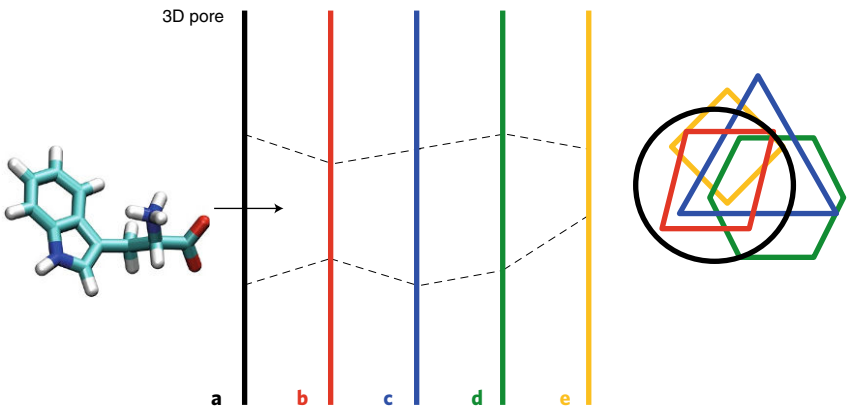


Fig. 2 | Schematic of a molecule passing through a 3D nanopore (illustrated by the dashed line) constructed of multiple layers. Each layer (labelled as a, b, c, d, e) can have different chemistry, pore size, position and other parameters. Right inset shows the left side view presenting the stacks of those layers with different pore shapes.

pathway, we can explore, in analogy to 3D integrated electronic circuits, the possibility of using the third dimension along such layered nanopores. In nanofluidics, this expansion can be, for example, exploited for a precise recognition, in a 'lock and key' manner, of the passing atomic and molecular species, in complete analogy to biological nanopores. For example, when different types of nanopores (catalogued distributions) are formed in each layer of graphene stacks, the parameters of a 3D nanopore would vary from layer to layer. Such a 3D composite nanopore would better match the sequence of groups present on the passing molecular species, in analogy to protein channels. Figure 2 shows a scheme of a 3D nanopore with atomically thin layers of different chemistries, pore sizes, positions and other parameters, where 3D molecular structures can be recognized. With the pores in individual layers displaced from the common longitudinal axis in a helical manner[8], the 3D nanopores can recognize the chirality and, potentially, other symmetry and chemical patterns of the passing molecules, due to more recognition elements being present along the channel lengths.

As an alternative perspective, methods of synthetic chemistry are likely to be used to prepare materials with atomically precise, complex nanopores that have properties matching different applications[9]. With these bottom-up (rather than top-down etching) methods, identical molecular components can be synthesized and covalently bound like LEGO into covalent (COF) and metal–organic frameworks (MOF) with perfectly periodic porous 2D and 3D architectures, respectively[10]. The overall chemistries, sizes, shapes and positions of such nanopores should be the same, giving the same local material properties throughout the whole structures. Based on the accurate information of nanopore configurations, the characteristics of such nanoporous materials can be optimized by self-learning methods, reminiscent of artificial intelligence approaches used in face recognition and self-driving cars. ❐

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