磁铁中心之旅

超高分辨率质谱，终于绘制出来了！

剧本：KanKr
绘图：Damour

Pierre Giusti is a PhD in analytical chemistry, head of the TRTG separation and molecular identification service at TotalEnergies and Director of Research at the CNRS, he is co-founder and director of the iC2MC joint laboratory. He is interested in the molecular characterization of complex matrices in the field of energy and its decarbonation. He is a specialist in analytical sciences for TotalEnergies.

Brice Bouyssiere is a professor of analytical chemistry at the institute of analytical sciences and physical chemistry for environment and materials (University of Pau and Adour Countries / CNRS), his research focuses on the characterization of complex matrices and development of hyphenated techniques between separation device and detection techniques. He is also Vice President Science with and for the society and open science at UPPA and co-founder and co-director of the iC2MC joint laboratory.

Carlos Afonso is a professor of analytical chemistry at the COBRA laboratory (Université de Rouen/ CNRS/INSA), his research focuses on developments in ultra-high resolution molecular mass spectrometry and ion mobility spectrometry. He is particularly interested in ionization and activation methods, especially for highly complex organic mixtures characterization. He is deputy director of the CNRS Infranalytics research infrastructure, in charge of the FTICR division, and is co-founder and co-director of the iC2MC joint laboratory.

Ryan Rodgers is a PhD in analytical chemistry and researcher at the National High Magnetic Field Laboratory (Florida State University), he is one of the world specialists in very high resolution mass spectrometry (FTICR MS). His research focuses on the characterization of complex matrices by FTICR MS. He is co-founder and co-director of the iC2MC joint laboratory and holds the international chair of High Resolution Mass Spectrometry at UPPA.

Julien Maillard is a PhD in analytical chemistry, he is a research engineer in the high-resolution mass spectrometry laboratory of TotalEnergies in Gonfreville. He is interested in the molecular characterization of complex matrices in the field of new energies.

Mélanie Mignot Mélanie Mignot obtained her PhD in analytical chemistry in December, 2016 and spent one year as temporary assistant professor at IUT Rouen in 2017. In 2017-2018, she received a MSCA Postdoctoral Fellowship in KU Leuven and in 2019, she became assistant professor and since 2023, associate professor at COBRA laboratory, INSA Rouen. Her current research areas include the instrumental and/or methodological developments, especially by chromatography hyphenated with high resolution mass spectrometry, for environmental or energy applications.

Attracted to science since childhood, after my high school diploma, I pursued a degree in geology before continuing my studies with a Master's in Communication and Scientific Culture at Grenoble. After graduating, my first job took me to Pau, where I began contributing to the journal Ebullition(s) as a SAPS mediator at the CCSTI Laqc Odyssée - Science Odyssée. Today, deeply committed to the project, I continue to work on the journal alongside my role as a scientific mediator in the Var.

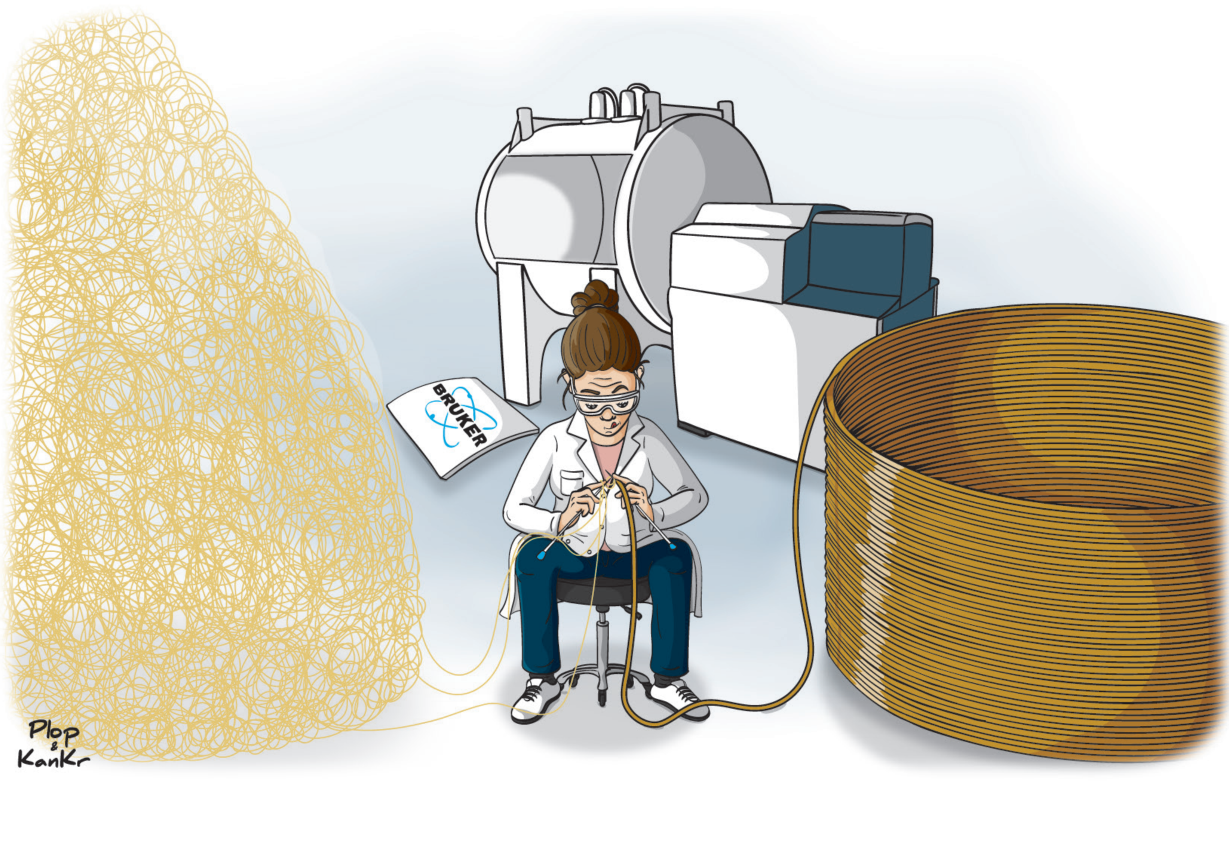
SUPER SPECTROMETER ARRIVES IN IC2MC LABS

Santa Claus is a little early this year. After weeks of loud noises, drilling, and pouring of a thick concrete slab for support, he's finally delivered the present...

In Rouen, Normandy, the COBRA laboratory has just installed a FT-ICR mass spectrometer equipped with an 18-tesla (T) magnet (the 2nd highest field in the world), i.e. around 1,800 times stronger than the magnetic field created by a fridge magnet. In parallel, at the Université de Pau et des Pays de l'Adour, in southern Aquitaine, as well as at the Gonfreville l'Orcher site of TotalEnergies research laboratories, received its little brothers, two 12 T's, which have just been installed as well. These three instruments complete iC2MC's fleet of FT-ICR MS instruments, along with the 21 T already in place at Florida State University's National High Magnetic Field Laboratory (NHMFL). But what's the point of these long-awaited high magnetic field machines in these 4 laboratories?

These devices are very high-resolution, high-precision, mass spectrometers. They can analyze and identify the individual components present in a complex sample. Unlike other mass spectrometers, these particular models contain extremely powerful superconducting magnets. They have large metal coils made of an alloy of niobium and titanium, several hundred kilometers in length, each weighing several tons. When an electric current flows through a coil, it produces a magnetic field, but would also emit heat - the Joule effect. However, when the coil is cooled to -269°C using liquid helium, it becomes superconducting, i.e. its electrical resistance becomes zero, and it no longer emits heat. This makes it possible to use an electric current of over 200 A to create a magnet with a very high magnetic field. Under these cold conditions, the huge coil is a superconducting magnet that produces a very stable and powerful magnetic field for science. But the technology doesn't stop there!

Known by its full name, Fourier Transform Ion Cyclotron Resonance Mass Spectrometer (or FT-ICR MS), this instrument performs mass spectrometry by combining the use of



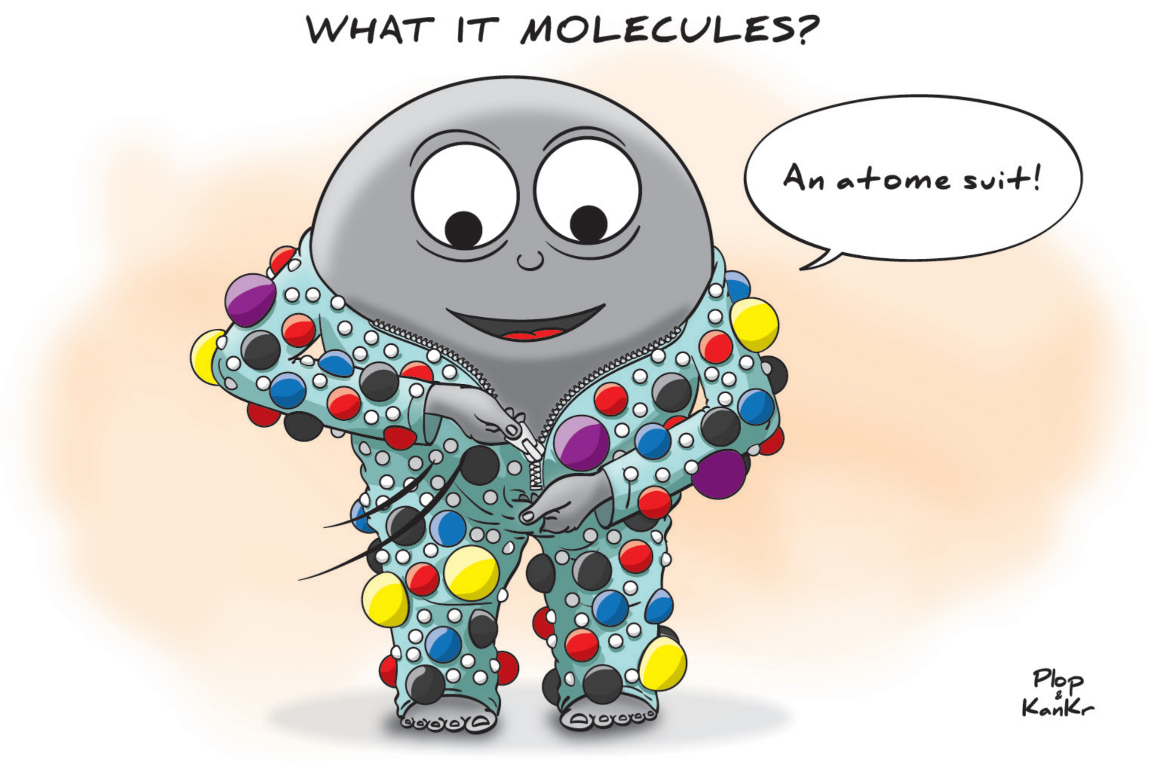
the superconducting magnet with a mathematical operation called the Fourier transform.

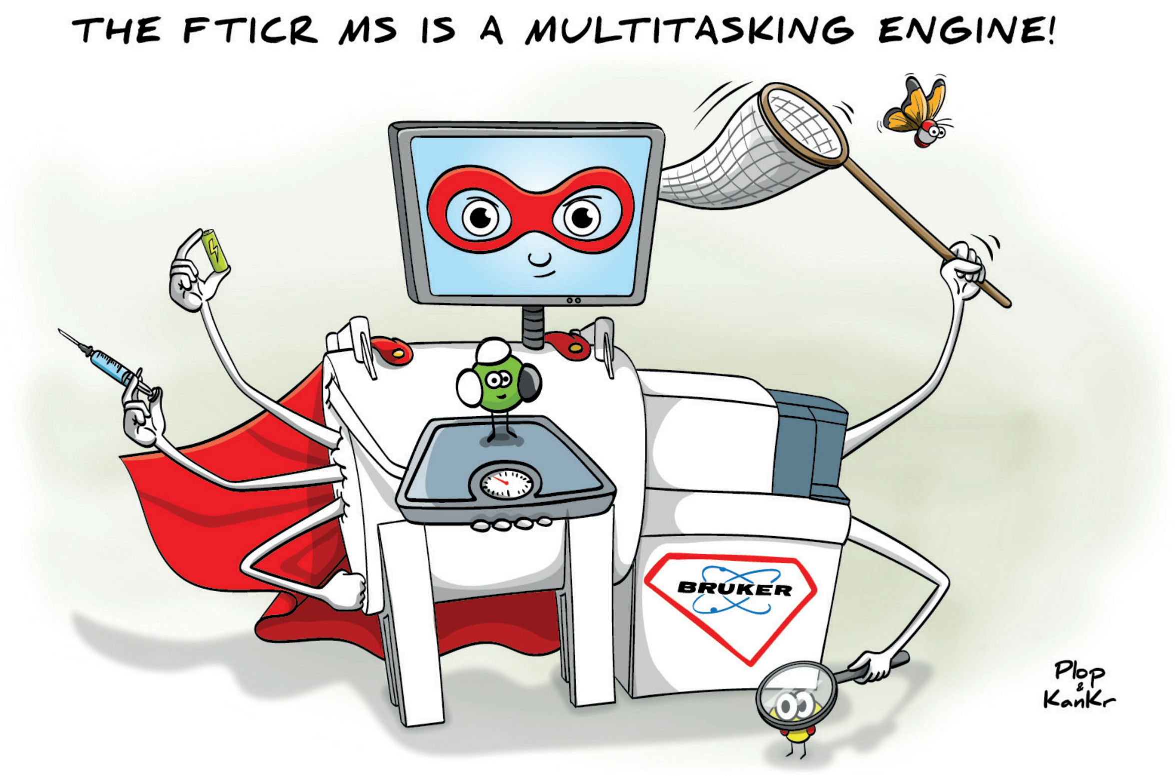
Invented by Marshall and Comisarow at the University of British Columbia in 1974, this instrument is used to study molecules, i.e. combinations of atoms. A molecule is made up of several atoms linked together by chemical bonds. Each molecule has a mass, corresponding to the sum of the masses of its constituent atoms. The aim of this super spectrometer is to measure the mass of molecules with the utmost precision, in order to elucidate their molecular composition. In addition, this instrument has a very high resolution, i.e. it is capable of separating molecules whose masses are very close (less than a single electron), which is essential for the analysis of very complex samples made up of tens of thousands of different molecules.

STATE-OF-THE-ART TECHNOLOGY

Thanks to its high dynamic range, this instrument can detect molecules present in a mixture, even in very small quantities. Furthermore, the high measurement accuracy of this instrument makes it very easy to determine the molecular formula of each molecule that makes up our sample, i.e. determining which types of atoms they contain, and how many of each type! Whereas an imprecise instrument would only provide molecular masses with a single digit after the decimal point, a FT-ICR spectrometer gives a value with 7 digits after the decimal point! This drastically reduces the possible atomic combinations for a given mass. This distinction is also made possible by the fact that the error, i.e. the difference between the theoretical mass and the experimentally measured mass, is less than 1 ppm (parts per million). This means that the measured error rate is less than 1 for every million units measured, making this super spectrometer one of the most accurate measuring instruments available!

At the same time, the very high field strength of the magnet gives the device a resolution of well over a million. Such high resolution enables very fine signals to be obtained, enabling molecules with very similar masses to be differentiated. With complex mixtures such as soils or combustion fumes containing





tens of thousands of molecules, the need for resolution is paramount.

This instrument enables us both to separate each molecule in a highly complex mixture and to assign a molecular formula to each signal, thus deciphering the molecular composition of a sample. It's a bit like wearing glasses for a short-sighted person... The contours are much sharper, more precise, and we're able to distinguish the details of an object and not just its overall shape.

HOW DOES IT WORK IN PRACTICE?

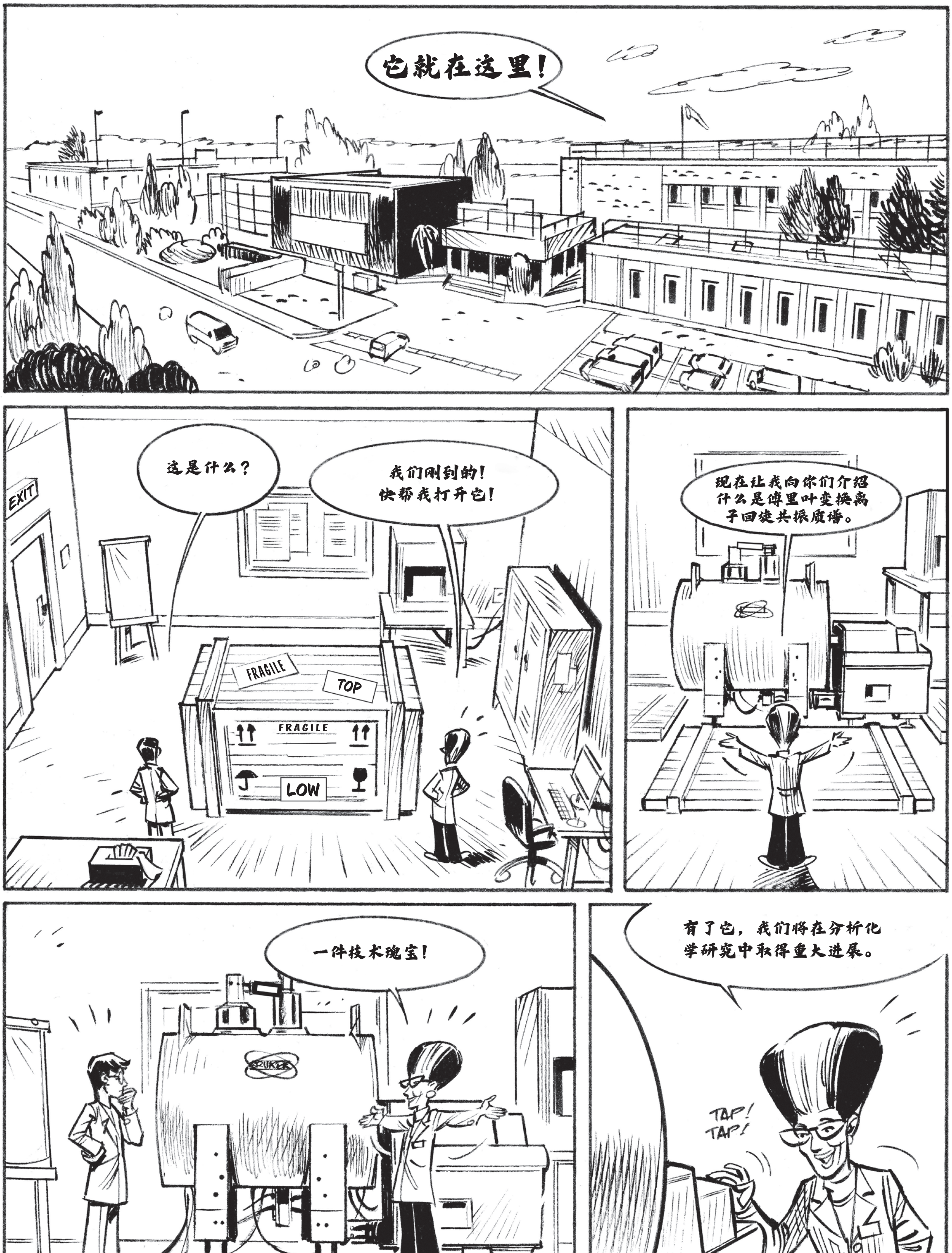
To begin with, you need to dilute the sample in a solvent. This is a bit like diluting grenadine in water, so that it's not too sweet. Next, the sample is introduced into the ionization source using a syringe. Naturally, a molecule is electrically neutral; it has no charge. But we can add charges to it, for example, by associating it with other charged species in the sample, so that our molecule becomes an ion. This step is important because the electric and magnetic fields used by the instrument would not be able to act on molecules without an electric charge, and the analysis would not work. Once the molecules have been ionized, the great journey begins, all the way to the heart of the spectrometer. Once in the center of the magnet, the ions will spin and travel tens of kilometers! But for the measurements to go smoothly, they must not encounter any obstacles, which is only possible in a very high vacuum corresponding to 13 orders of magnitude less than atmospheric pressure! To achieve this, the instrument is equipped with very powerful vacuum pumps called turbomolecular pumps.

To determine the mass of ions, we measure their rotational frequency, which depends on their mass. By applying a mathematical operation known as the Fourier transform, it is possible to determine the frequency of each ion, enabling us to calculate their mass using a very simple calculation.

Of course, for this to work at its best, expert users must be able to optimize the acquisition parameters to ensure optimum ion transmission, and the instrument must be very well calibrated to obtain highly accurate measurements. To achieve this, reference molecules with known masses are used.

The instrument generates a huge amount of data. To manage this data more easily, the international laboratory iC2MC (International Complex Matrices Molecular Characterization) has developed software capable of determining molecular formulas and representing the data obtained in the form of molecular maps, to facilitate comparison between samples.

These new spectrometers will enable us to push back the boundaries of molecular characterization and explore in greater detail highly complex samples in the healthcare, energy and environment sectors, and many others!


它就在这里！
这是什么？
我们刚到的！
快帮我打开它！
EXIT
FRAGILE
TOP
FRAGILE
LOW
现在让我向你们介绍
什么是傅里叶变换离
子回旋共振质谱。
一件技术瑰宝！
有了它，我们将在分析化
学研究中取得重大进展。
TAP!
TAP!


它可以帮助我们解决超级复杂样本的分析问题，了解它们的分子组成，甚至可以检测到某些痕量化合物。
并检测到以前看不到的成分。
它可以识别到世界上所有存在的物质。
C22 H31 N3 Zr
此外，这台机器具有非常大的动态范围，可以同时看到复杂样本中的高浓度组分和那些痕量组分。
我们一直在等您来。
它可以区分数百万种分子。

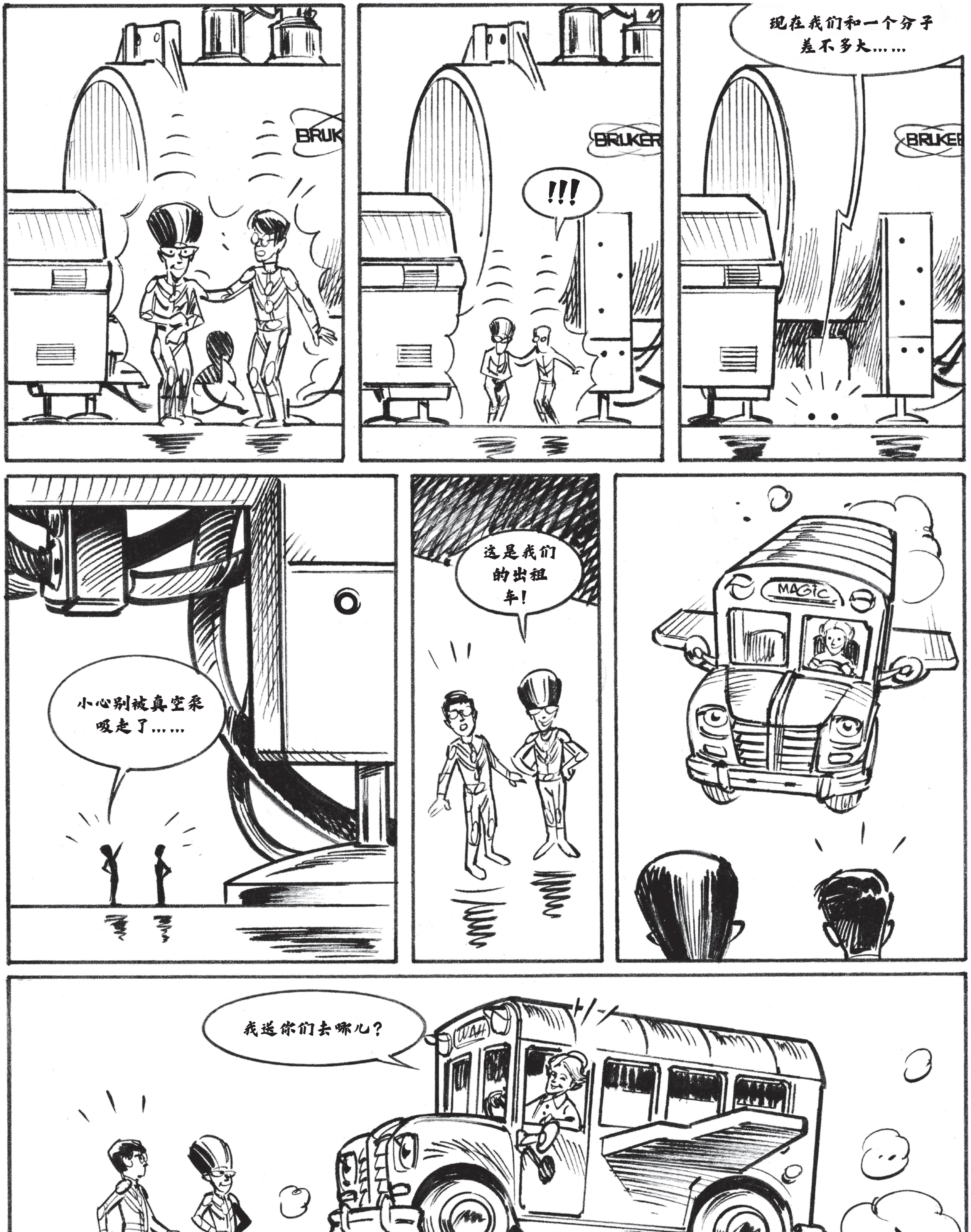

一个分子是由多个原子组成。
现在让我一个人静一静！！！
由于分子的原子组成不同，每个分子都有一个特定的质量。
我不应该吃甜点的……
使用质谱仪就可以测试出它的"实际"质量。
因此，这测量精度可是大事儿！如果天平不准或者有偏差，就会直接影响分子的鉴定结果。
EXIT

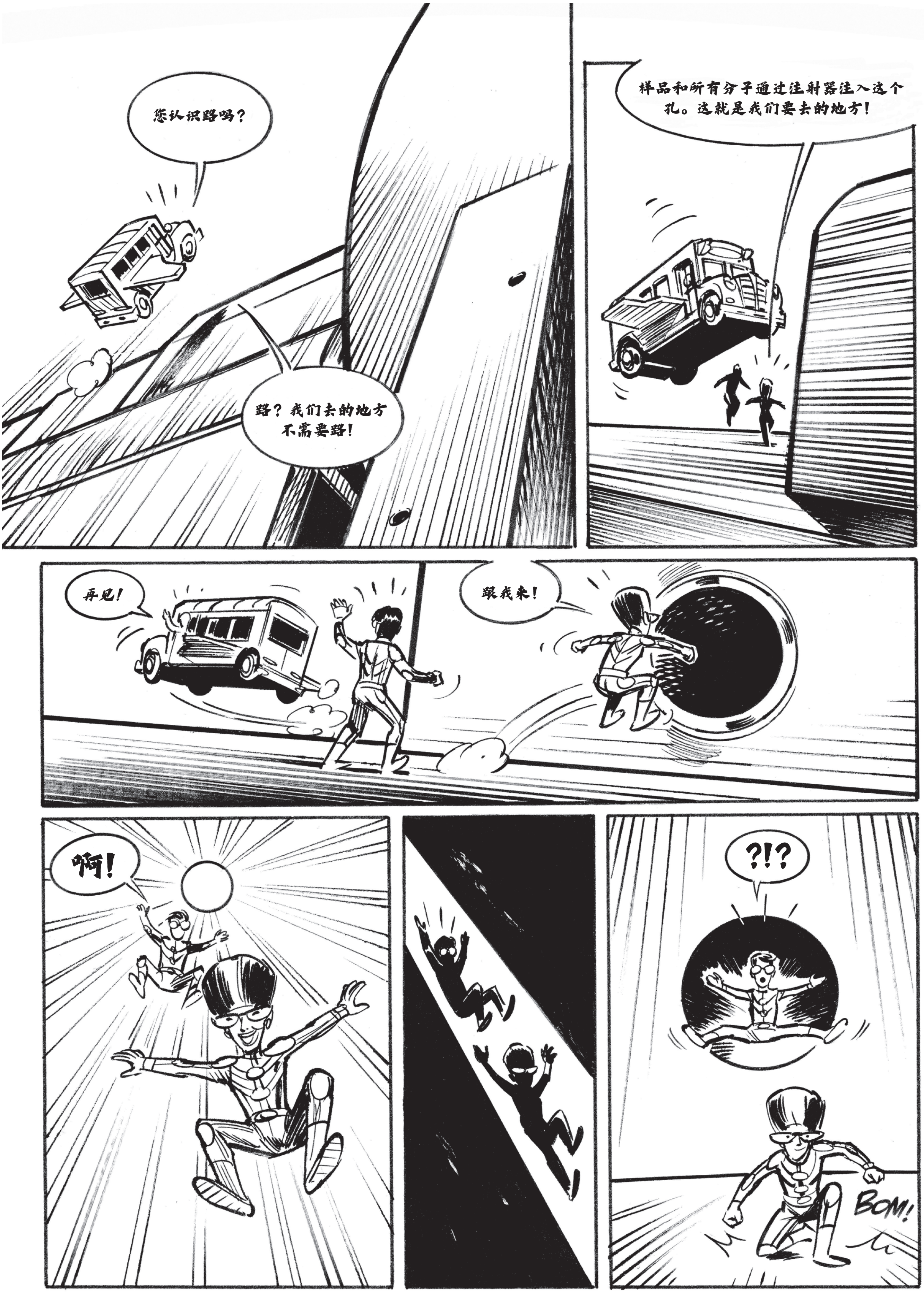

382道尔顿
不精确
1道尔顿（DA）=
1克每摩尔
382,25574
道尔顿
非常精确
质谱仪的测量精度取决于其测量观察到的质量小数值的能力。
使用这一台仪器，分子量测试得会非常准，可以直接给出分子式，拿到分子量对应的分子组成。
哇塞，这质谱仪简直就是个超级侦探，它那锐利的眼睛能看透到小数点后面好几位，把那些微小的差别都给揪出来！
嗯……
怎么了？
事情没那么简单……


分子自己是很难移动的，然而，要想称量它，首先我们要把它放在天平上……
我……来……了……
这次我们要称量的东西比一粒沙子还要轻数百亿亿倍！
因此，必须首先将分子转化为离子。
EXIT
要将分子转化为离子，我们必须使其带负电或正电。
这就是所谓的电离！
Creating an ion...
- e⁻
+ H⁺


在这里我们有两种电离方法。
J.FENN的电喷雾法，适用于液体样品，以及K.TANAKA的激光解吸附电离法，用于分析固体表面上的分子。
HIGH VOLTAGE
TAYLOR CONE
NEBULIZATION CONE
LASER SOURCE
MATRIX MIXTURE
IONS
IONIZATION
DESORPTION
J. FENN
NOBEL PRIZE IN CHEMISTRY 2002
K. TANAKA
NOBEL PRIZE IN CHEMISTRY 2002
这里就是样品引入后离子化发生的地方。
在这里，分析物失去一个电子或者得到一个质子，或者与其它带电物质结合从而产生离子。
最后，这里就是魔法发生的地方。
在这里，离子被称量。仪器会根据它们的质量和电荷将这些离子区分开。
简而言之，它们被分类了！
跟我来，我带你去看一下！

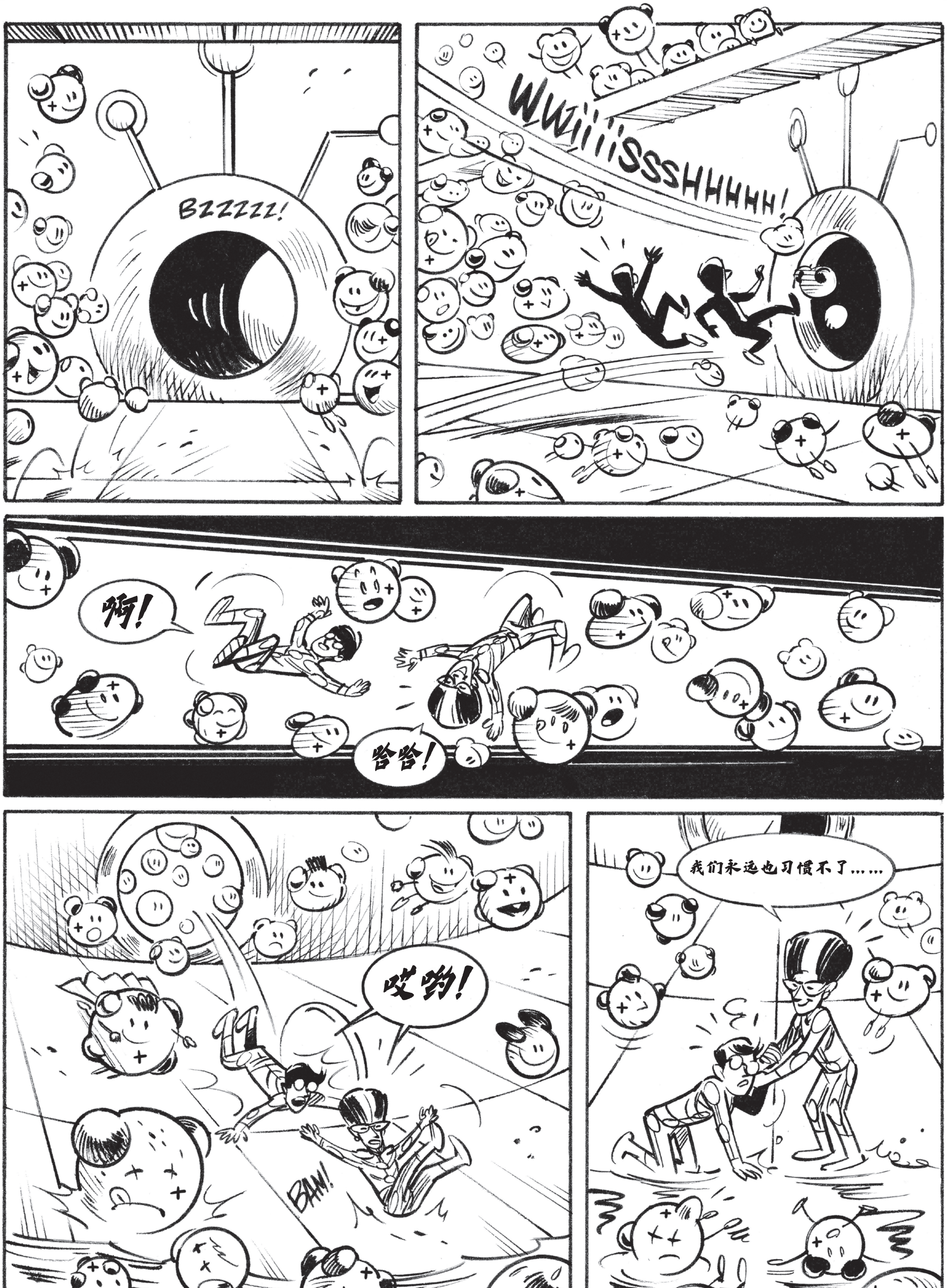

HONEY, I SHRUNK THE KIDS
Alan Marshall
NOBELS
穿上这个!
NOBELS
把手放在我的肩膀上。
BRUKER
减少原子间的距离!
?
BIIIP!

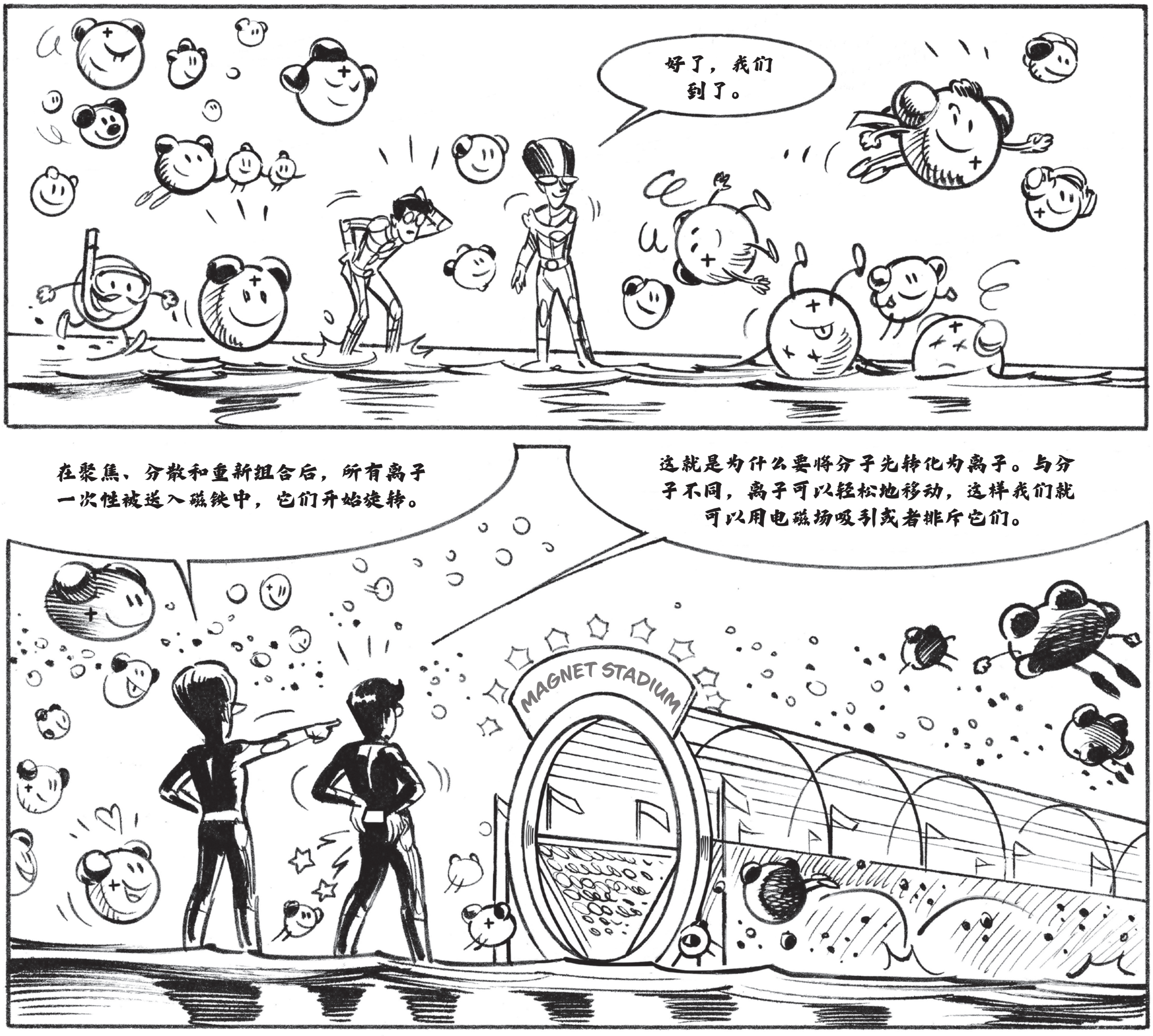

!!!
现在我们和一个分子差不多大……
小心别被真空泵吸走了……
这是我们的出租车！
我送你们去哪儿？

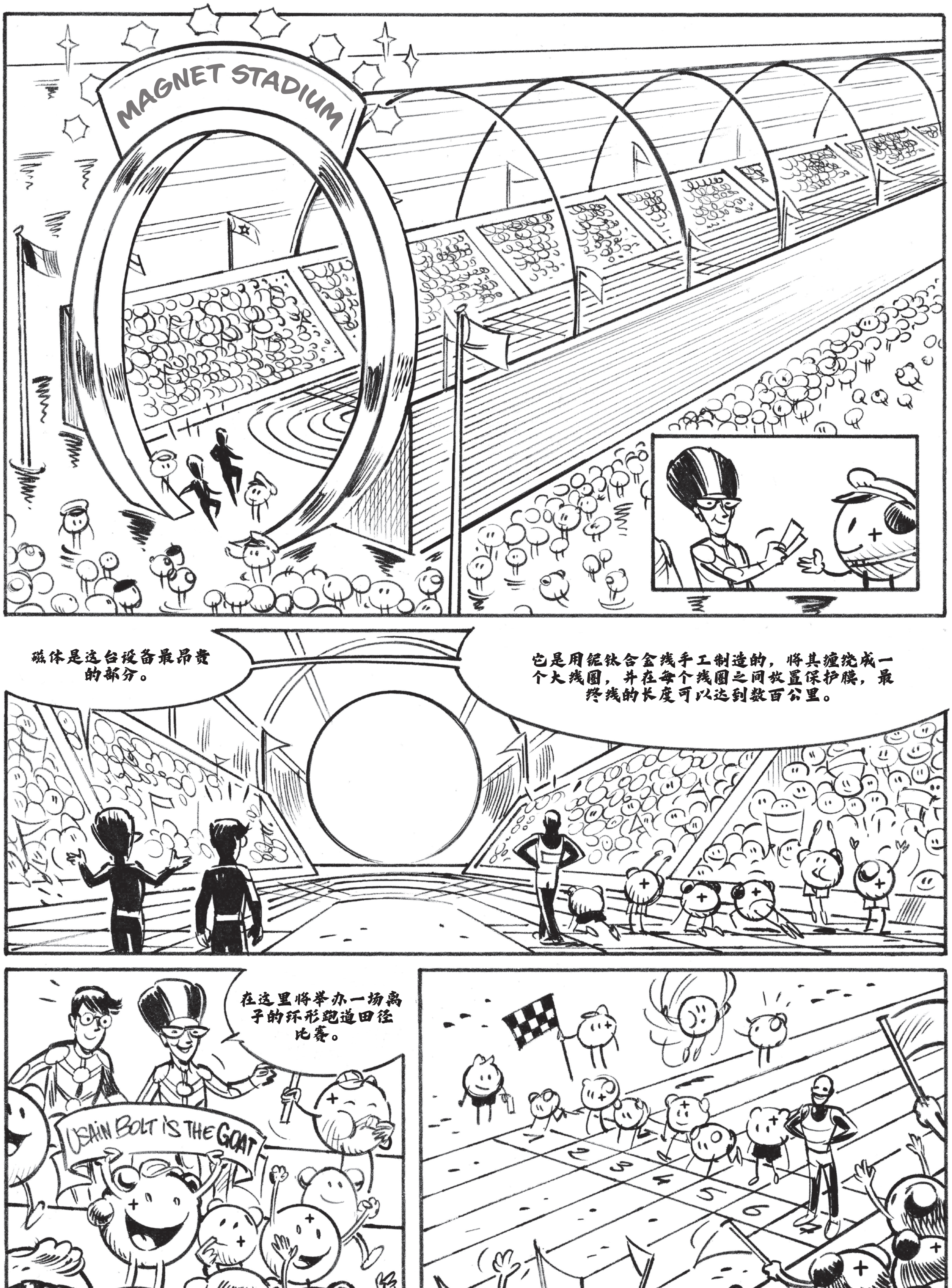


您认识路吗？
路？我们去的地方不需要路！
样品和所有分子通过注射器注入这个孔。这就是我们要去的地方！
再见！
跟我来！
啊！
?!?
BOM!


这里是一切开始的地方！
在这个大候车室里，所有的分子都在等待着。
一滴样品中的分子比撒哈拉沙漠中的沙粒还多。虽然不是所有分子都被电离，但每滴样品中仍有数十亿个分子！
一旦分子带电，它们就会等待进入下一个房间，在那里一切都会发生。
这扇门后面在发生什么？
你很快就会知道了……

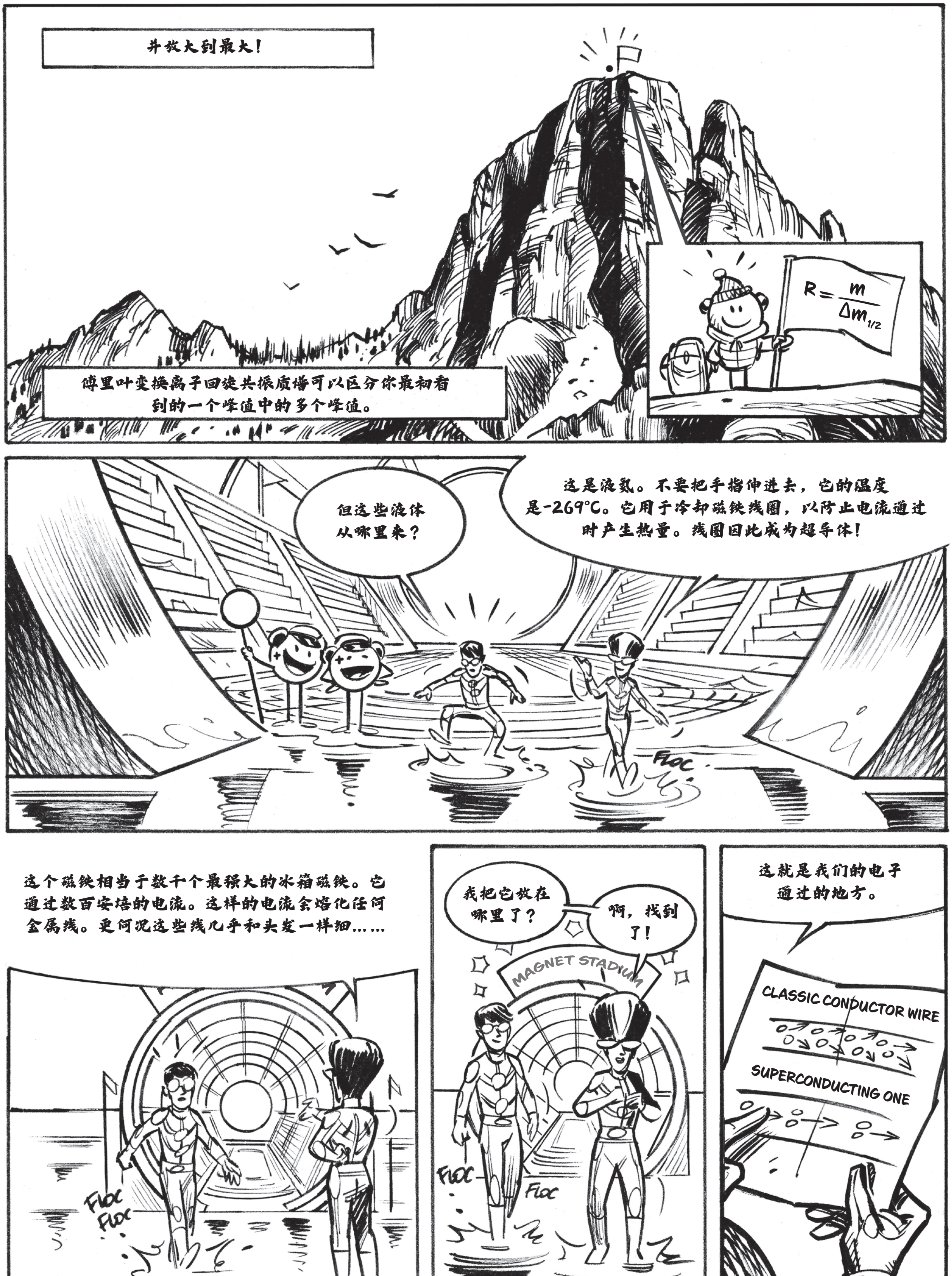

BZZZZZ!
WWiiiiSSSHHHHHH!
啊!
爸爸!
哎哟!
BAM!
我们永远也习惯不了……

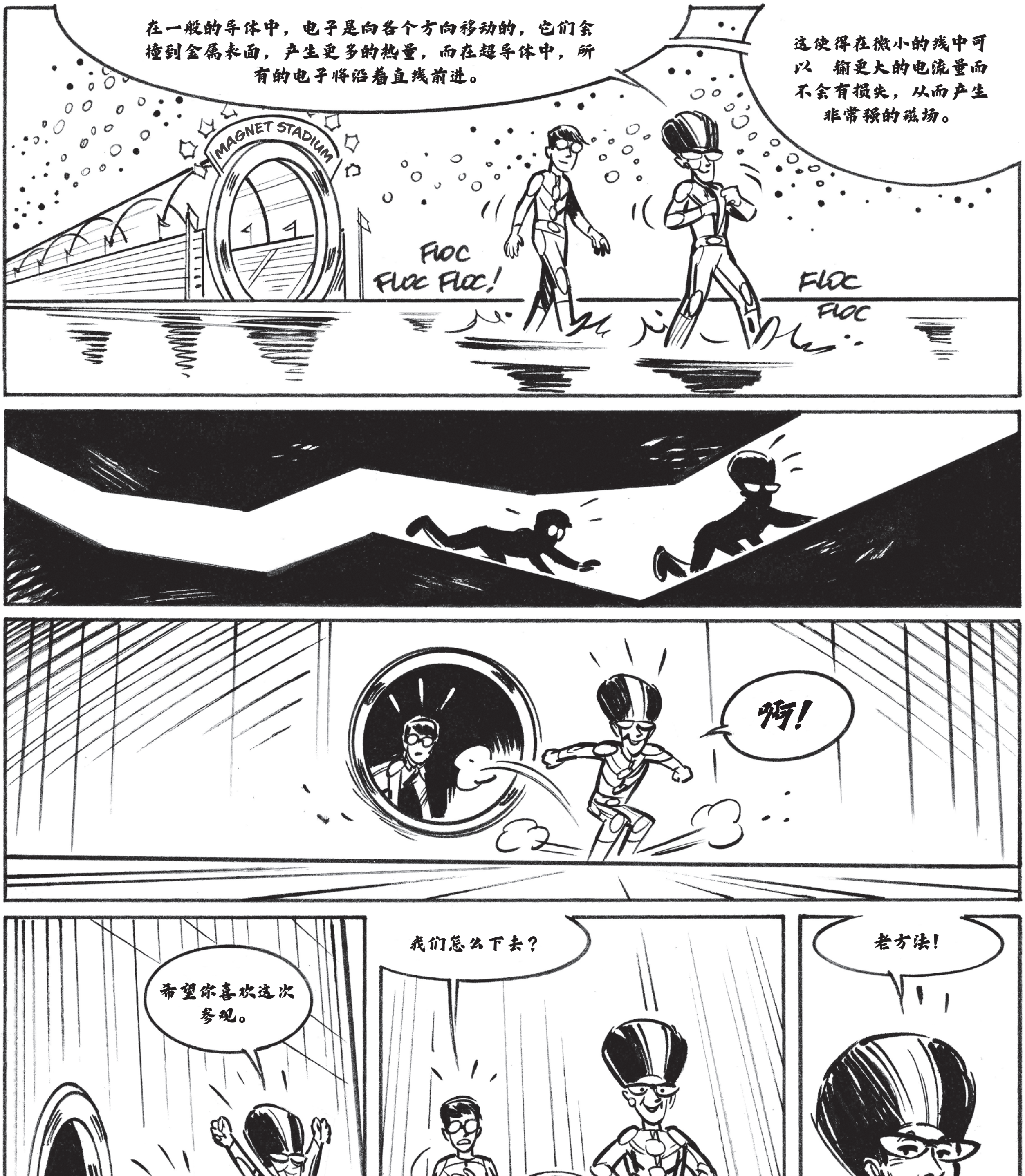

好了，我们到了。
在聚焦、分散和重新组合后，所有离子一次性被送入磁铁中，它们开始旋转。
这就是为什么要将分子先转化为离子。与分子不同，离子可以轻松地移动，这样我们就可以用电磁场吸引或者排斥它们。
MAGNET STADIUM
没错！当我们将离子置于磁场中时，它会围绕磁场轴旋转。这种旋转的周期性取决于其质量、电荷和磁场强度。
离子的回旋共振！
比赛即将开始……
让我们近距离看看！

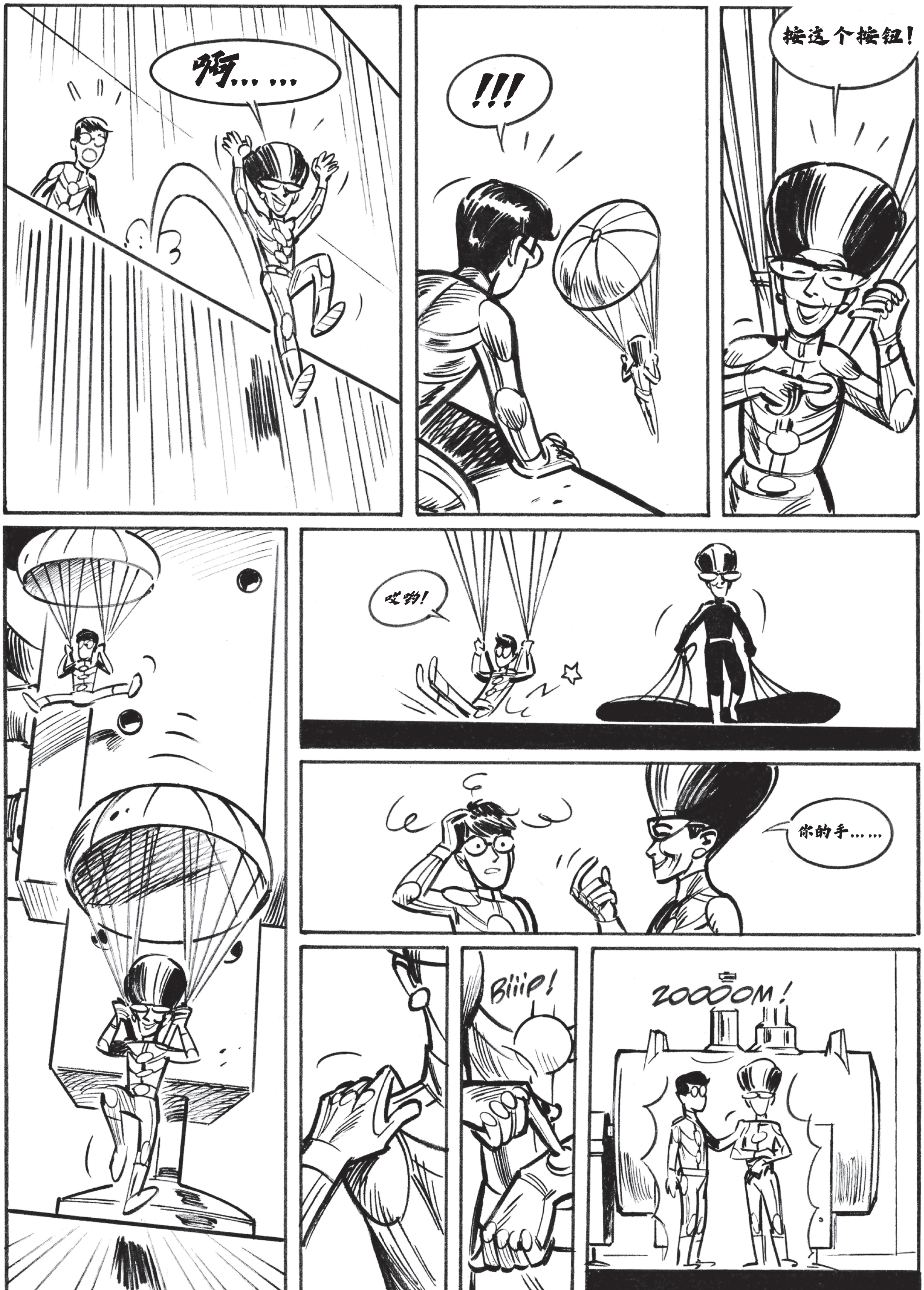

MAGNET STADIUM
磁体是这台设备最昂贵的部分。
它是用铌钛合金线手工制造的，将其缠绕成一个大线圈，并在每个线圈之间放置保护膜，最终线的长度可以达到数百公里。
在这里将举办一场离子的环形跑道田径比赛。
USAIN BOLT IS THE GOAT
1
2
3
4
5
6


这就是为什么不能随便开始比赛，所有人都必须在相同的时间点起跑。
离子的质量是根据它绕赛道一圈所需的时间获得的，经过大量圈数后测量其旋转频率。
!!!
PAN!
根据磁体的大小，离子在被测量前跑的距离相当于从巴黎到马赛。
在超导磁体的帮助下，磁场强度可以一直保持稳定，因此离子的旋转频率（OMEGA）直接决定了离子的质量。
Z
ZZZ
我们测量得到的回旋频率，经过一种称为傅里叶变换的数学方程的转换，最终得到离子的质量。
换句话说……
Z
Z
这就是我们面前的傅里叶变换离子回旋共振质谱仪：FTICR MS。
$m = \frac{q \cdot B_0}{\omega_c}$


目前，市场上有几种磁场强度，7特斯拉或12特斯拉，此外，还有更高磁场强度的磁体。
有什么区别呢？
磁体的大小。如果磁体是相同的，所有离子的旋转方式相同。磁体强度越高，能同时参加比赛的离子就越多，它们跑的距离也越长。
它们旋转得越多，我们就能将它们分离得越开，从而区分质量非常接近的两个分子。这就是所谓的分辨率。
这有点像用肉眼看南奥索峰……
然后，用双筒望远镜……

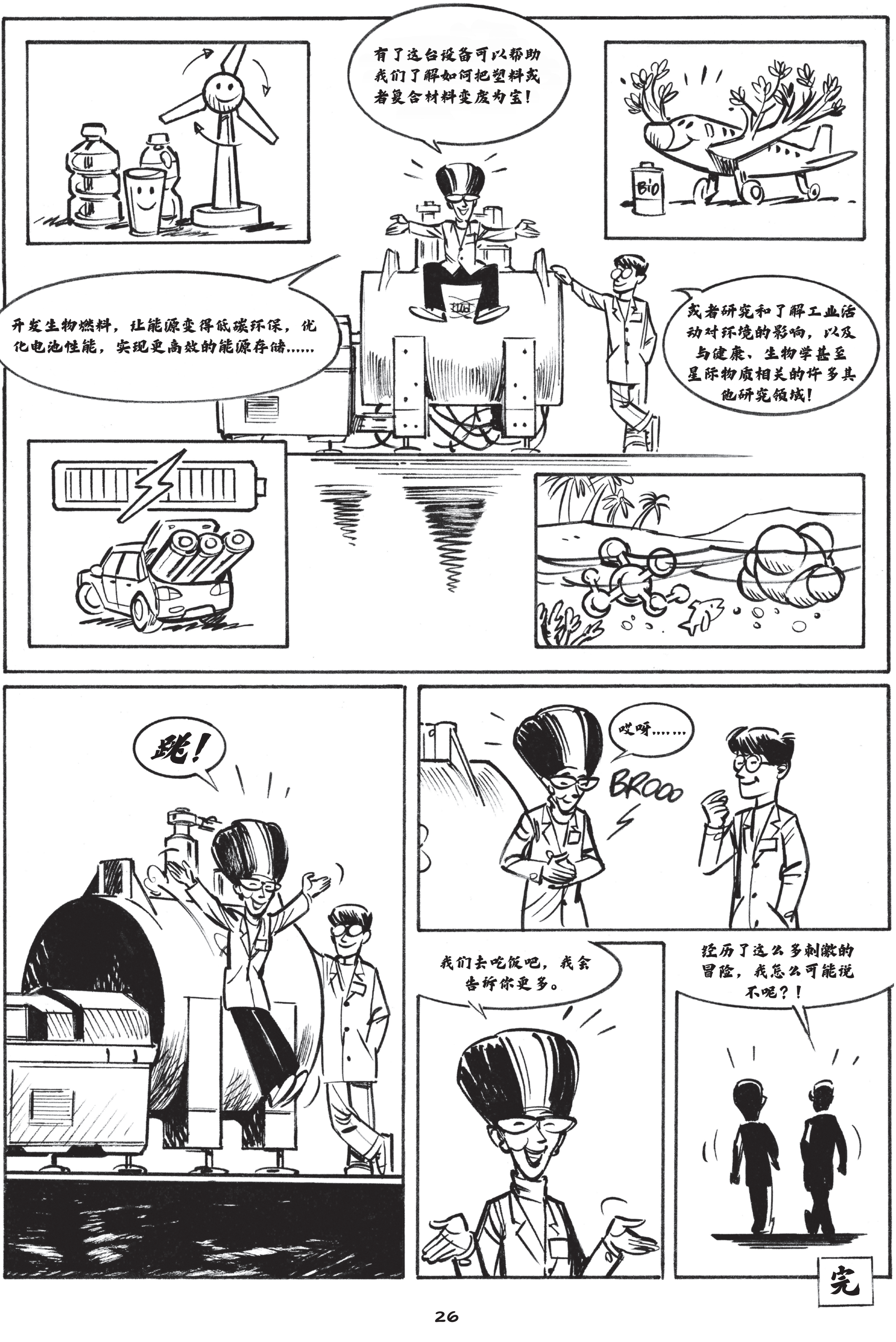

并放大到最大！
$R = \frac{m}{\Delta m_{1/2}}$
傅里叶变换离子回旋共振质谱可以区分你最初看到的一个峰值中的多个峰值。
但这些液体从哪里来？
这是液氦。不要把手指伸进去，它的温度是-269°C。它用于冷却磁铁线圈，以防止电流通过时产生热量。线圈因此成为超导体！
FLOC
这个磁铁相当于数千个最强大的冰箱磁铁。它通过数百安培的电流。这样的电流会熔化任何金属线。更何况这些线几乎和头发一样细……
FLOC FLOC
我把它放在哪里了？
啊，找到了！
MAGNET STADIUM
FLOC
FLOC
这就是我们的电子通过的地方。
CLASSIC CONDUCTOR WIRE
SUPERCONDUCTING ONE


在一般的导体中，电子是向各个方向移动的，它们会撞到金属表面，产生更多的热量，而在超导体中，所有的电子将沿着直线前进。
这使得在微小的线中可以 输更大的电流量而不会有损失，从而产生非常强的磁场。
MAGNET STADIUM
FLOC FLOC FLOC!
FLOC FLOC
呵!
希望你喜欢这次参观。
我们怎么下去？
老方法!



啊……
!!!
按这个按钮!
哎哟!
你的手……
Biiip!
ZOOOOM!


这是一项圆满完成的任务呀！
嗯……
还不完全……
现在，我们需要处理数据。
我们需要获取离子比赛的结果，给出它们的质量，将获得的质量汇总到一个表格中，并添加它们各自的强度……
……将这些质量与原子组成进行比较，从而找出它们对应的是什么。
PyC2MC
我们还有一整晚的工作要做！
TAP! TAP!
开玩笑呢，电脑会自动处理这些数据，我们已经编写了相应的代码，只需要在最后检查一下是否有错误就可以了！



有了这台设备可以帮助我们了解如何把塑料或者复合材料变废为宝！
开发生物燃料，让能源变得低碳环保，优化电池性能，实现更高效的能源存储……
或者研究和了解工业活动对环境的影响，以及与健康、生物学甚至星际物质相关的许多其他研究领域！
Bio
跳！
哎呀……
BROOO
我们去吃饭吧，我会告诉你更多。
经历了这么多刺激的冒险，我怎么可能说不呢？！
完

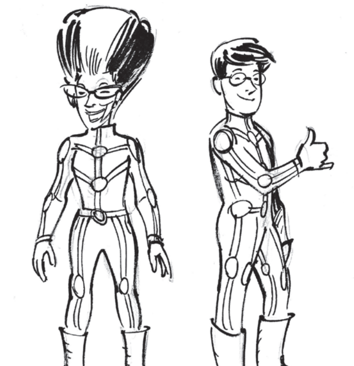
KanKr, whose real name is Simon Baert, is an author. He is the scriptwriter of the duo Plop & KanKr, formed with the cartoonist Julie Besombes, alias Plop. Together, they regularly publish in regional, national, and international press (*Le Monde, Siné Mensuel, Le Temps, Sud Ouest dimanche, Le Sans-culotte 85, L'Anjou Laïque, La Galipote, La Gazette du Béarn des gaves*...) and on television (Une semaine dans le monde on France 24). They are members of the Cartooning for Peace and Cartoon Movement networks. He also scripts scientific popular comics for the University of Pau and the Pays de l'Adour within the framework of the Science with, and for Society label.

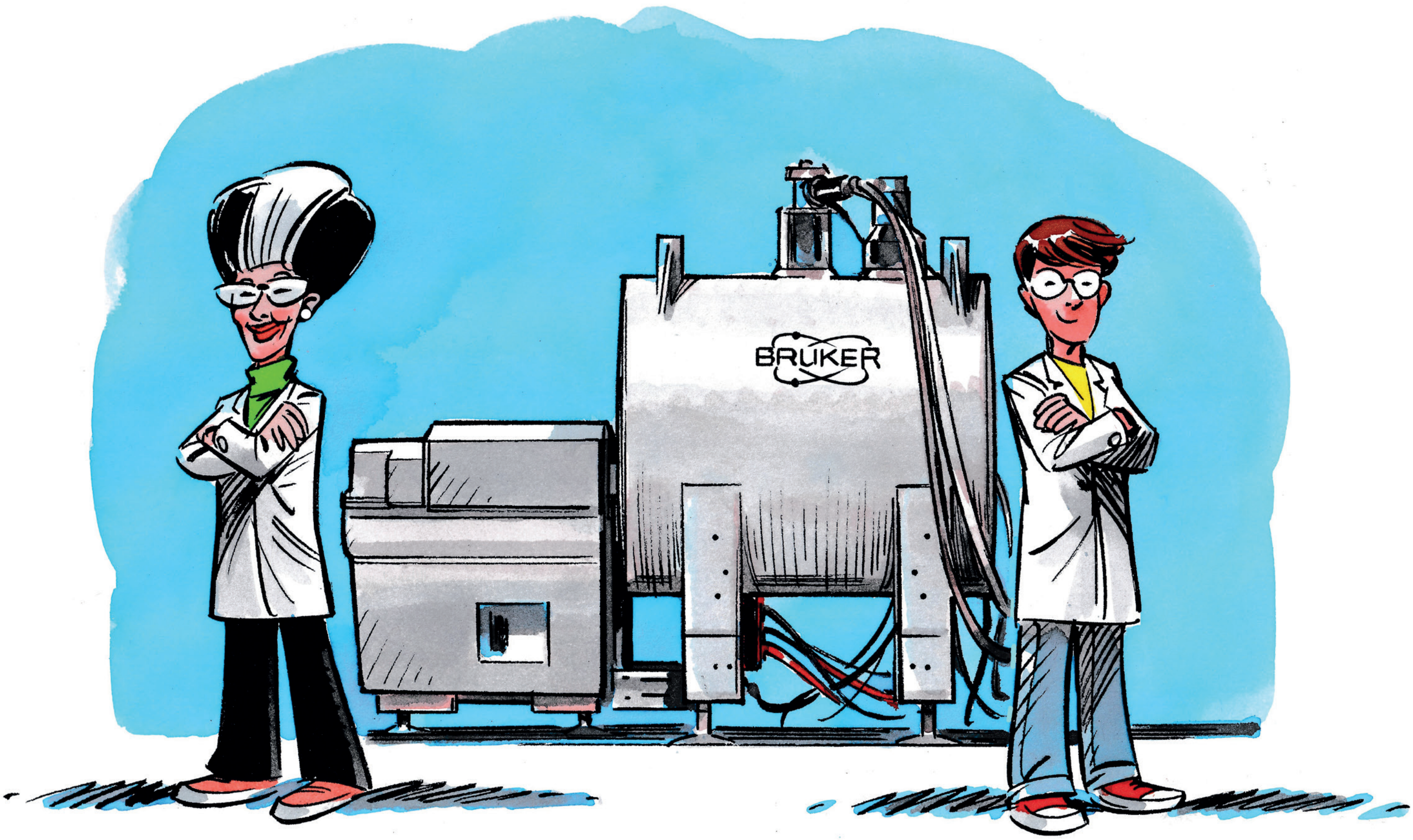
Sébastien Tessier signs his comic books under the pseudonym **DAMOUR**, his mother's maiden name. Born in La Roche-sur-Yon in 1972, a passionate amateur of drawing, he came to study plastic arts in 1990 in Bordeaux where he still resides. He decided to live from his passion for comics and met Delcourt Editions at the Angoulême fair in 1994. This was the beginning of a long collaboration with the scriptwriter Jean-Pierre Pécau on the series *Nash* and *Le Testament du Docteur M*. He has produced 28 albums to date, with various scriptwriters and illustrators, including the series *Pinkerton, La Cagoule, un Fascisme à la française* at Glénat, as well as two historical albums, *Kennedy* with Sylvain Runberg as scriptwriter and *L'Etincelle de Saint-Sardos*, of which he is the author, at Sud-Ouest editions. He is passionate about history and has been working on historical projects for several years.

Plop, whose real name is Julie Besombes, is a press cartoonist, illustrator and graphic designer. Together with KanKr, she forms the duo Plop & KanKr, who publish in the regional, national and international press (*Le Monde, Siné Mensuel, Le Temps, Sud Ouest dimanche, Le Sans-culotte 85, L'Anjou, Laïque, La Galipote*...) and for television (Une semaine dans le monde on France 24). She also produces press cartoons and popular science cartoons for the University of Pau and the Pays de l'Adour as part of the Science with and for Society label Science avec et pour la société.

Cai Jiao Ping is a teacher of Chinese and French. As an interpreter and translator, she teaches at the University of Pau and the Adour Region (UPPA), the Confucius Institute of Pau Pyrénées, and the University of Free Time of Aquitaine. She trains future language teachers in the French as a Foreign Language (FLE) program and conducts workshops and numerous seminars. Additionally, as a self-employed professional, she shares Chinese culture through courses for all ages and audiences..

Thomas Ferreira is editor and graphic designer at Presses universitaires de Pau et des pays de l'Adour (PUPPA). In particular, he helped to create the comic strip magazine *Ebullition(s)*, for which he is artistic director. He is also an illustrator and graphic designer under the name Atelier Decafé.





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