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A FAIR road to a bioAFM databank

Jean-Luc Pellequer^{1§*}, Sebastian Aguayo², Andrea Alessandrini³, David Alsteens⁴, Toshio Ando⁵, Audrey Beaussart⁶, Michael Betton⁷, Timo Betz⁸, Kerstin G. Blank⁹, Simone Bovio¹⁰, Clément Campillo¹¹, Claudio Canale¹², Alexander X. Cartagena-Rivera¹³, Filomena A. Carvalho^{14, 15}, Ignacio Casuso^{16§}, Guillaume Charras¹⁷, Marti Checa¹⁸, Liam Collins¹⁸, Adai Colom¹⁹, Luca Costa²⁰, Etienne Dague²¹, Tanya E.S. Dahms²², Pedro Jose de Pablo²³, Alexandra Delvallée^{24§}, Simone Dinarelli²⁵, Lorna Dougan²⁶, Yves F. Dufrêne²⁷, Andra C. Dumitru⁴, Yuri M. Efremov²⁸, Sofiane El-Kirat-Chatel⁶, Paolo Facci²⁹, Georg E. Fantner^{30§}, Amir Farokh Payam³¹, Cécile Feuillie⁶, Cristina Flors³², Nancy Forde³³, Cécile Formosa-Dague³⁴, Gregory Francius³⁵, Clemens M. Franz³⁶, Kristian Franze³⁷, Ricardo Garcia³⁸, Sergi Garcia-Manyes³⁹, Núria Gavara⁴⁰, Marina I. Giannotti⁴¹, Marco Girasole²⁵, Martin Guthold⁴², George R. Heath^{43§}, Céline Heu⁴⁴, Peter Hinterdorfer⁴⁵, Jamie K. Hobbs⁴⁶, Bart W. Hoogenboom^{47§}, Sébastien Janel^{48§}, Miklós Kellermayer⁴⁹, Petr Klapetek⁵⁰, Noriyuki Kodera⁵, Melanie Köhler⁵¹, Frank Lafont⁴⁸, Guillaume Lamour¹¹, Jessem Landoulsi⁵², Valérie Laurent⁵³, Philippe Leclère⁵⁴, Malgorzata Lekka⁵⁵, Hongbin Li⁵⁶, Giovanni Longo²⁵, Arin Marchesi⁵⁷, Marion Mathelié-Guinlet⁶, Gerald A. Meininger⁵⁸, Ioanna Mela⁵⁹, Pierre-Emmanuel Milhiet²⁰, Ruben Millan-Solsona¹⁸, Tea Misic Radic⁶⁰, Michaël Molinari⁶, Fernando Moreno-Herrero⁶¹, Michael A. Nash⁶², Olivier Noël⁶³, Yoo Jin Oh⁴⁵, Laia Pasquina-Lemonche^{64§}, Shivprasad Patil⁶⁵, Patricia Pedraz³², Ana Paula Pêgo⁶⁶, Thomas T. Perkins⁶⁷, Martin Pesl⁶⁸, Tri Thanh Pham⁶⁹, Laura Picas⁷⁰, Alessandro Podestà^{71§}, Johannes Preiner⁷², Jan Přibyl⁷³, Roger Proksch⁷⁴, Pierre-Henri Puech⁷⁵, Alice L. B. Pyne^{76§}, Manfred Radmacher⁷⁷, Lorena Redondo^{16§}, Felix Rico^{16§}, Wouter H. Roos^{78§}, Robert Ros⁷⁹, Nuno C. Santos^{14, 15}, Ugis Sarkans^{80§#}, Tilman E. Schäffer⁸¹, Hermann Schillers⁸², Zhifeng Shao⁸³, Delphine Sicard⁸⁴, Adam Cohen Simonsen⁸⁵, Igor Sokolov⁸⁶, Susana R. Sousa⁸⁷, Bjørn T. Stokke⁸⁸, Andreas Stylianou⁸⁹, Marek Szymonski⁹⁰, Florence Tama⁹¹, Neil H. Thomson⁹², Takayuki Uchihashi⁹³, Massimo Vassalli⁹⁴, Claude Verdier⁵³, Anthony Vial⁶, Véronique Vié⁹⁵, Tomaso Zambelli⁹⁶, Renato Zenobi⁹⁷, Peng Zheng⁹⁸, and Claire Valotteau^{16§*}

§ Members of the initial working group on AFM databank; # represented by Sameer Velankar

*Corresponding authors

The 2020s are characterized by the proliferation of artificial intelligence (AI), a development that, while not novel, has been propelled by the recent accessibility of vast quantities of data. To pursue this avenue, it is of the utmost importance to create high-quality, open databanks. A number of biophysical communities are concurrently engaged in the development of their respective databanks and databases. In this commentary, we aim to direct attention toward the initial efforts to establish a high-quality databank with atomic force microscopy (AFM) data: bioAFM-DB. There are encouraging signs within the community suggesting a shift toward depositing AFM data in public repositories. This commentary outlines the current state of this endeavor, its challenges, and potential courses of action.

40 Databanks are repositories that gather and store scientific data, thereby enabling the development
41 of databases that facilitate the organization and retrieval of this data. Public repositories have
42 existed for more than 50 years, long before the advent of “Big Data.” One of the oldest repositories in
43 the molecular biology field is the Protein Data Bank (PDB), which emerged from a handful of
44 crystallographers in 1971.¹ Databanks evolve based on available computational infrastructure and
45 changes in the global needs of the research community. Currently, the Registry of Research Data
46 Repositories (re3data.org) contains over 3,300 repository sites^{Suppl. ref 1}, some of which are related to
47 “Microscopy”. For instance, the registry includes extensions of the PDB, such as the Nucleic Acid
48 Knowledgebase;² specialized resources, such as the Yeast Resource Center Public Image Repository³
49 and the Brain Image Library;⁴ and general image repositories, such as the Image Data Resource,⁵ and
50 the BioImage Archive.⁶ Some microscopy-related repositories manage electron microscopy (EM) data,
51 such as the Electron Microscopy Data Bank,⁷ which stores electron density maps, and the Electron
52 Microscopy Public Image Archive,⁸ which provides raw images and 3D cryo-EM maps.

53 Currently, there is no repository for scanning probe microscopy (SPM). SPM is a family of microscopy
54 techniques^{Suppl. ref 2} derived from the scanning tunneling microscope (STM), which was developed in the
55 early 1980s^{Suppl. ref 3}. A prevalent member of the SPM family, atomic force microscopy (AFM)⁹ was
56 developed in 1986 and has become widespread in both material and biological sciences^{Suppl. ref 4}. AFM
57 detects a sample surface with a sharp probe integrated at the end of a flexible cantilever, which allows
58 a spatial topographic map to be obtained at nanoscale resolution and physical properties to be
59 measured^{Suppl. ref 5}. Key benefits of using AFM in life science applications over other types of
60 microscopies include the ability to image biological samples in physiological buffer conditions (i.e., in
61 liquid and at a controlled temperature) and an exceptional signal-to-noise ratio, which enables imaging
62 individual molecules with sub-nanometer resolution in topography^{Suppl. ref 6}. Moreover, AFM allows
63 probing physical properties of biological samples, including active biomolecules, proteins, nucleic
64 acids, biomaterials, living cells and tissues, and obtain stiffness, adhesion or viscosity maps^{Suppl. ref 7}.
65 Development of faster scanning AFM technologies has allowed imaging of biological processes and

66 biomolecular dynamics down to sub-nanometer spatial and sub-second temporal resolutions^{Suppl. ref 8}.
 67 In this commentary, we advocate for establishing a path towards the creation of a bioAFM databank
 68 (bioAFM-DB) and the development of its associated databases.

69 Is now the right time to develop a repository for AFM data? We believe so because AFM has reached
 70 a level of maturity and use that was not the case 20 years ago^{Suppl. ref 9}. Specifically, in the last 10 years,
 71 among the average yearly 9000 published articles containing “Atomic Force Microscop*” topics, only
 72 9.2% contained AFM, or its explicit name, in their titles, indicating that it has become a routine
 73 biophysical tool. Other signs of maturity include the availability of high-quality, free and open-source
 74 software for handling AFM data, such as WsXM^{Suppl. ref 10}, Gwyddion^{Suppl. ref 11}, AtomicJ^{Suppl. ref 12},
 75 FiberApp^{Suppl. ref 13}, SmarTrace^{Suppl. ref 14}, Nanite^{Suppl. ref 15}, Topostats^{Suppl. ref 16}, AutoSmarTrace^{Suppl. ref 17},
 76 dForce2.0^{Suppl. ref 18}, PyFMLab^{Suppl. ref 19}, NanoLocz^{Suppl. ref 20}, CellMAP^{Suppl. ref 21}, and a growing population of
 77 AFM analysis scripts at GitHub^{Suppl. ref 22, ref 23}. Furthermore, there is a continuous increase in applications
 78 using AFM data in structural biology such as AFM-Assembly^{Suppl. ref 24}, BioAFMViewer^{Suppl. ref 25},
 79 Trace_y^{Suppl. ref 26}, and recently with high-speed AFM films such as tools based on rigid-body fitting^{Suppl.}
 80 ^{ref 27, ref 28} and flexible fitting^{Suppl. ref 29, ref 30} via normal mode analysis NMFF-AFM^{Suppl. ref 31}, NanoLocz^{Suppl. ref}
 81 ²⁰, BioAFMViewer 5.0^{Suppl. ref 32}, and AFMFit^{Suppl. ref 33}. Another incentive for the timing of an AFM data
 82 repository is the recent ambition of research institutions and funding agencies to encourage
 83 researchers to find, access, interoperate, and reuse scientific data.

84 Both the USA National Science Foundation (NSF) and the National Institutes of Health (NIH) mandate
 85 data sharing as a core expectation of federally funded research. In 2016, the European Commission
 86 established the FAIR Data Principles, FAIR being an acronym for Findable, Accessible, Interoperable,
 87 and Reusable.¹⁰ These principles establish guidelines that go beyond the common practice of including
 88 statements such as "data is available upon request" in publications. The FAIR principles aim at
 89 correcting shortcomings in data availability, including missing or incomplete data descriptors, rigid or
 90 non-standardized file formats, a lack of data organization and validation, and low persistence of data

91 over time^{Suppl. ref 34}. The FAIR principle acknowledges the effort involved in producing data and the
92 global economy surrounding data access and storage within the research community. The importance
93 of data archiving has been extensively discussed^{10,11,Suppl. ref 35}. Multiple scientific fields are progressing
94 in the FAIR definition of their data such as NMR-based metabolomics data^{Suppl. ref 36}, optical tweezers¹²
95 and biomolecular simulations.¹³ The benefits of data archiving include physical access to raw data,¹⁴
96 which is often different from the processed data found in the supplementary materials of published
97 articles. Data archiving fosters reproducibility in research, conserves taxpayer resources by eliminating
98 redundant research, and maintains public confidence in science. Undoubtedly, the most significant
99 benefit of publicly accessible data is accelerating scientific discoveries by building on available data
100 beyond its original purpose. A paradigmatic example of this is the above mentioned PDB, whose
101 founders may not have anticipated successful reutilization of their data in the prediction tools like
102 AlphaFold2^{Suppl. ref 37} and RoseTTAFold^{Suppl. ref 38} when depositing their experimentally determined X-ray
103 structures. We, as researchers developing and applying AFM to biological and biomolecular systems
104 co-signing this commentary, agree on the importance of distributing AFM data and support this effort.

105 AFM data sharing would require a certain level of standardization regarding data acquisition, storage
106 and annotation. Several proactive standardization actions should be mentioned. As early as 2010, the
107 issue of AFM data management was raised within a European network on applications of atomic force
108 microscopy to nanomedicine and life sciences (COST Action TD1002). This Action proposed a
109 Standardized Nanomechanical Atomic force microscopy Procedure (SNAP) that improved
110 reproducibility of elasticity measurements^{Suppl. ref 39}. Earlier round-robin experiments pointed towards
111 similar standardized calibration of AFM cantilevers^{Suppl. ref 40}. The SNAP approach was further improved
112 during the Marie Skłodowska-Curie Innovative Training Network Phys2BioMed, by including sample
113 preparation and data analysis standardized routines^{Suppl. ref 41}. Also developed during the Phys2BioMed,
114 effort in standardization continued with a tentative definition of a common text-based AFM universal
115 file format^{Suppl. ref 19, ref 42}. Additional efforts include the establishment of a dataset of simulated-AFM
116 images of small organic molecules^{Suppl. ref 43} or the recent development of a structural biology-

117 compatible file format for AFM^{Suppl. ref 44}. In short, an AFM databank should store the experimental raw
118 AFM data, its accompanying metadata and its related processing steps to improve the reproducibility
119 in this field.

120 Therefore, why does an AFM databank not already exist? The daunting procedural tasks required for
121 developing a strategy to deposit AFM data in a public repository may answer this question. One major
122 hurdle in creating an AFM databank is the wide variety of samples and associated preparation
123 protocols as well as heterogeneity of data types. AFM crosses a range of fields, from physics and
124 chemistry to biology. There is an enormous number of sample types, ranging from mineral materials
125 to biological tissues, from hard to soft specimens, and from conductive to insulating surfaces. This
126 variety of samples correlates with a wide range of measurement modes, from topographic images to
127 force measurements. There is also the possibility of datasets from AFM systems coupled, for example,
128 to optical microscopes^{Suppl. ref 45} or infrared^{Suppl. ref 46} and Raman^{Suppl. ref 47} spectroscopies. Thus, defining
129 the minimum metadata for all these types of samples and information requires a significant effort.
130 Furthermore, there are several AFM instrument manufacturers, including laboratories building their
131 own instruments, each with several models and various levels of historical legacy in their data formats.
132 The FAIR principles cannot be applied to these proprietary formats; therefore, most data from AFM
133 instruments cannot be stored in a database without prior conversion and without a reading tool that
134 ensures interoperability (as found in AFMReader^{Suppl. ref 48}, for instance). Another issue raised by the
135 community concerns data quality, as there are no clear definitions of what constitutes good and bad
136 topographic images or force-distance curves. This issue requires an open discussion among the AFM
137 communities.

138 In retrospect, a possible reluctance to distribute AFM data may originate from a lack of understanding
139 of how and for what "others" who did not produce the data might use it. For instance, a particular
140 group may want to test its developed data processing tools on AFM data from other laboratories. For
141 that, multiple images or force-distance curves of different quality (good, fair, or poor) would be

needed. It is, however, unusual that a scientific publication necessitates the deposition of “poor quality” AFM data. A clear advantage of a databank should be the deposition of complete datasets, rather than a couple of images or force curves included in published works.

To fulfill the FAIR principle, the bioAFM data repository must adhere to the following constraints:

1) A robust infrastructure is required to upload, store and distribute the data (FA).

2) A specific ontology should be agreed upon to prepare the minimum informative metadata, both human and computer readable (I).

3) Deposited data should contain the minimum information necessary to reproduce and analyze the data; including functional/dedicated open software (IR).

4) Data quality must be appropriately annotated (FIR)

Where do we stand now? Fortunately, the maturity of the AFM field means that this project does not have to start from scratch. A group of volunteers has started working on this AFM metadata. The group officially met before and during the AFM data symposium, which was held alongside the 15th AFMBioMed conference, in Barcelona in April 2025, and advanced in dividing the metadata into subsections: sample, cantilever, experimental conditions, recording parameters and data. The European Bioinformatics Institute (EBI) of EMBL generously oversees these preliminary metadata efforts and is committed to following the development process for the potential integration of the AFM database into the EBI. The EBI's contribution is invaluable to our community because it provides the necessary infrastructure for data deposition, finding, access, dissemination, and visualization. One clear benefit of collaborating with the EBI is its expertise in providing time-based data access through appropriate release.

The development of a databank is an ambitious long-term project. While the initial design strategies should be as broad as possible, it is impractical to start the project with every type of AFM data. The

166 project will progress in steps to grow into a full-scale repository. Following the positioning of the EBI
167 in the field of life sciences, the "bio" side of the databank will develop first, and the immediate focus
168 will target three AFM data types: topography, spectroscopy, and nanomechanics. Volunteers are
169 welcome and encouraged to join this initiative by contacting the corresponding authors, and
170 contribution not only from academia but also from the industrial sector will be essential. In addition
171 to the minimal metadata required for deposition, two major topics need further discussion:

172 1) What constitutes a dataset or a databank entry?

173 Several questions arise: which of the experimentally recorded data should be stored in the database?
174 Should the data be linked to a scientific publication? Can large datasets be stored as a single entry?
175 Should all recorded data be deposited or just the relevant data used in the associated publication? Let
176 us take the example of AFM topography. Depending on the experimental imaging mode, several kinds
177 of data are recorded simultaneously, also known as channels (deflection, height, amplitude error,
178 phase signal). Most often with AFM height images, if we ignore the trace and retrace measurements,
179 only a single channel (height) is used. Should it be the only deposited data? Should the accompanying
180 measurements and calibrations be also deposited? How to handle the tip convolution effect in AFM
181 topography? All these details will be discussed and evaluated during the course of establishing this
182 databank and its underlying databases. There is nevertheless a topic of importance for initial
183 deposition in the databank: reference datasets (images, pulling, indenting). These datasets are
184 especially important for standardization efforts in research and in metrology. They should allow for
185 poor-quality, noisy, and diverse AFM measurements of realistic AFM data, which may be valuable for
186 developers of novel AFM data processing tools. In the era of artificial intelligence and machine-
187 learning, the need for extremely large, diverse, and accurately annotated datasets has become even
188 more pressing^{Suppl. ref 9}. Training robust models requires not only raw data but also high-quality ground-
189 truth labels, which are scarce, labor-intensive to generate, and often inconsistent across laboratories.
190 As a starting point, since many journals have policies that require data deposition, the initial data

191 deposited in the repository could likely be that included in submitted manuscripts. However, there is
192 plenty of room for discussion.

193

194 2) Defining the architecture and format of the AFM data files in the repository to allow conversion
195 from a proprietary format to the open repository's format and their import/export tools.

196 Although any specific data format can be deposited in a databank, a lack of a common format will
197 reduce the effectiveness of AFM data dissemination, both inside and outside the AFM community. It
198 highlights the particular role of file conversion and reading software tools, such as those from
199 Gwyddion^{Suppl. ref 11}, afmformats^{Suppl. ref 15}, Topostats^{Suppl. ref 16}, AFMReader^{Suppl. ref 48}, NanoLocz^{Suppl. ref 20}
200 and PyFMReader^{Suppl. ref 19}. The development of an integrative AFM file format has already begun, as
201 demonstrated by the Universal Spectroscopic and Imaging Data (USID) format developed at the Oak
202 Ridge National Laboratory^{Suppl. ref 49} or the UFF mentioned above^{Suppl. ref 19}. A possible starting point is to
203 deposit raw AFM data and include a tool for exporting and downloading raw data to transform it into
204 manageable data, as AFMReader does. Once again, as a community, it will be important to reach an
205 agreement about a common AFM data exchange file format.

206 Our ultimate goal is to promote a unified platform, in the spirit of the PDB,¹ to all AFM communities.
207 We will have fulfilled part of our goals if we reach the following three objectives: 1) Disseminate
208 bioAFM data in various biological fields beyond the laboratories that produce it; 2) Improve user
209 education on using bioAFM data, particularly regarding the associated pitfalls; 3) Increase the
210 integration of bioAFM data into other biophysical pipelines, such as integrated structural biology for
211 AFM topography. This platform will include an online AFM data deposition mechanism, appropriate
212 validation of depositions, and a referencing key, such as an entry code or digital object identifier (DOI).
213 In a second stage, improvements will involve interlinking with other databases such as MBDB,¹⁴
214 MechanoPro-DB^{Suppl. ref 50}, MechanoBase^{Suppl. ref 51}. A possible starting point could be the BioStudies
215 system at EBI.¹⁵ The bioAFM databank will be established through a governance framework that

216 defines usage policies and the ethical implications of using open data. We anticipate reaching a
217 significant milestone in this active development process at a symposium organized alongside the next
218 AFMBioMed conference, in Brno, in 2027.

219 **The development of bioAFM-DB and its related databases is poised to address open questions across**
220 **diverse fields—from single-molecule conformations and molecular binding mechanisms to the**
221 **mechanics of aging, and diseases. By making AFM findings accessible to broader scientific**
222 **communities, bioAFM-DB will enable cross-validation of experimental data with other microscopies**
223 **(such as EM and super-resolution) and biophysical tools (including optical tweezers and**
224 **nanoindenters), as well as with computational models. This integration will further establish bioAFM**
225 **as a standard tool in biophysics and exemplifies the transformative potential of merging biophysics**
226 **and data science, driving knowledge forward through a multidisciplinary approach.**

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261

262 **Affiliations:**

- 263 1. Univ. Grenoble Alpes, CEA, CNRS, IBS, F-38000 Grenoble, France.
- 264 2. School of Dentistry and Institute for Biological and Medical Engineering, Pontificia Universidad
265 Católica de Chile, Santiago, Chile.
- 266 3. Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia,
267 Italy and CNR-Nanoscience Institute-S3, Modena, Italy.
- 268 4. NanoBiophysics lab, Louvain Institute of Biomolecular Science and Technology, UCLouvain,
269 Louvain-La-Neuve, Belgium.
- 270 5. Nano Life Science Institute, Kanazawa University, Kanazawa, Japan.
- 271 6. Univ. Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, F-33600 Pessac, France.
- 272 7. Plateforme Nanobio LIPHY; MC2 group, Laboratoire Interdisciplinaire de Physique, 140 rue de
273 la physique, F-38400 Saint Martin d'Hères, France.
- 274 8. Third Institute of Physics – Biophysics, University of Göttingen, Germany.
- 275 9. Institute of Experimental Physics, Johannes Kepler University Linz, Austria.
- 276 10. Laboratoire de Reproduction et Développement des Plantes, Université de Lyon, Université
277 Claude Bernard Lyon 1, ENS de Lyon, Institut National de Recherche pour l'Agriculture,
278 l'Alimentation et l'Environnement (INRAE), CNRS, 69364 Lyon Cedex 07, France; and PLATIM-
279 LyMIC Univ Lyon, SFR Biosciences, ENS de Lyon, Inserm US8, CNRS UMS3444, UCBL - 50 Avenue
280 Tony Garnier, 69007 Lyon, France.
- 281 11. Université Paris-Saclay, Univ Evry, CY Cergy Paris Université, CNRS, LAMBE, 91025, Evry-
282 Courcouronnes, France.
- 283 12. Department of Physics, University of Genoa, Italy.
- 284 13. Section on Mechanobiology, National Institute of Biomedical Imaging and Bioengineering,
285 National Institutes of Health, Bethesda, MD 20892, USA.
- 286 14. GIMM – Gulbenkian Institute for Molecular Medicine, Lisbon, Portugal.
- 287 15. Faculdade de Medicina, Universidade de Lisboa, Lisbon, Portugal.
- 288 16. Aix-Marseille Univ, INSERM, DyNaMo, Turing centre for living systems, Marseille, France.
- 289 17. London Centre for Nanotechnology, University College London, London, UK, and Department
290 of Cell and Developmental Biology, University College London, London, UK.
- 291 18. Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge,
292 Tennessee 37831, USA.
- 293 19. Biofisika Institute (CSIC, UPV/EHU) and Department of Biochemistry and Molecular Biology,
294 University of the Basque Country, Leioa, Spain.
- 295 20. CBS (Centre de Biologie Structurale), Univ Montpellier, CNRS, INSERM, Montpellier, France.
- 296 21. LAAS-CNRS, CNRS, Université de Toulouse, Toulouse, France.
- 297 22. Department of Chemistry and Biochemistry, University of Regina, 3737 Wascana Parkway,
298 Regina, SK, Canada S4S 0A2.
- 299 23. Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain.
- 300 24. Laboratoire National de métrologie et d'Essais (LNE), Trappes, France.
- 301 25. Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Rome, Italy.
- 302 26. School of Physics and Astronomy, University of Leeds, UK.
- 303 27. Louvain Institute of Biomolecular Science and Technology, UCLouvain, Croix du Sud, 4-5, bte
304 L7.07.07, B-1348 Louvain-la-Neuve, Belgium.
- 305 28. Institute for Regenerative Medicine, Sechenov First Moscow State Medical University
306 (Sechenov University), 119991 Moscow, Russia.
- 307 29. Institute of Biophysics , National Research Council, Genova, Italy.
- 308 30. Interfaculty Institute for Bioengineering, École Polytechnique Fédéral de Lausanne,
309 Switzerland.
- 310 31. Nanotechnology and Integrated Bioengineering Centre, School of Engineering, Ulster
311 University, UK.

- 312 32. Madrid Institute for Advanced Studies in Nanoscience (IMDEA Nanociencia), Madrid, Spain.
- 313 33. Department of Physics, Simon Fraser University, Burnaby, BC, Canada.
- 314 34. TBI, Université de Toulouse, INSA, INRAE, CNRS, Toulouse, France.
- 315 35. INSERM – CNRS - Université de Strasbourg, UMRS 1121/EMR 7003, Strasbourg, France.
- 316 36. WPI NanoLSI, Kanazawa University, Japan.
- 317 37. Max Planck Zentrum für Physik und Medizin, Erlangen, Germany; Medical Institute of
318 Biophysics, FAU Erlangen-Nürnberg, Erlangen, Germany; Department of Physiology,
319 Development and Neuroscience, University of Cambridge, UK.
- 320 38. Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain.
- 321 39. Department of Physics & Randall Centre for Cell and Molecular Biophysics, King's College
322 London, UK.
- 323 40. Unit of Biophysics and Bioengineering, Department of Biomedicine, School of Medicine and
324 Health Sciences, Universitat de Barcelona, Barcelona 08036, Spain.
- 325 41. Department of Materials Science and Physical Chemistry and IQTC, University of Barcelona -
326 Institute for Bioengineering of Catalonia (IBEC), BIST - CIBER-BBN, ISCIII - Barcelona, Spain.
- 327 42. Department of Physics, 2090 Eure Drive, Wake Forest University Winston-Salem, NC 27109,
328 USA.
- 329 43. School of Physics and Astronomy, University of Leeds, Leeds, UK.
- 330 44. Katharina Gaus Light Microscopy Facility, Mark Wainwright Analytical Centre, UNSW SYDNEY,
331 Australia.
- 332 45. Institute of Biophysics, Johannes Kepler University Linz, Austria.
- 333 46. School of Mathematical and Physical Sciences, University of Sheffield, UK.
- 334 47. Nanosurf AG, Gräubernstrasse 12-14, 4410 Liestal, Switzerland; and London Centre for
335 Nanotechnology, University College London, 19 Gordon Street, London WC1H 0AH, United
336 Kingdom.
- 337 48. Univ. Lille, CNRS, Inserm, CHU Lille, Institut Pasteur de Lille, U1019 - UMR 9017 - CIIL - Center
338 for Infection and Immunity of Lille, F-59000 Lille, France.
- 339 49. Department of Biophysics and Radiation Biology, Semmelweis University, Budapest, Hungary.
- 340 50. Czech Metrology Institute, Okružní 31, 638 00 Brno, Czech Republic.
- 341 51. Leibniz Institute for Food Systems Biology at the Technical University of Munich, Freising,
342 Germany.
- 343 52. Sorbonne Université, CNRS, Laboratoire de Réactivité de Surface, LRS, F-75005 Paris, France.
- 344 53. Univ. Grenoble-Alpes, CNRS, LiPhy - Grenoble, F-38000, France.
- 345 54. University of Mons (UMONS)/Laboratory for Physics of Nanomaterials and Energy (LPNE),
346 Research Institute for Materials Science and Engineering, Place du Parc 20, B 7000 Mons,
347 Belgium.
- 348 55. Department of Biophysical Microstructures, Institute of Nuclear Physics, Polish Academy of
349 Sciences, Krakow, Poland.
- 350 56. Department of Chemistry, University of British Columbia, Canada.
- 351 57. Department of Experimental and Clinical Medicine, Università Politecnica delle Marche,
352 60126, Ancona, Italy.
- 353 58. Dalton Cardiovascular Research Center. Department of Medical Pharmacology and Physiology.
354 University of Missouri-Columbia, 134 Research Park Drive, Columbia, MO 65211, USA.
- 355 59. Department of Pharmacology, University of Cambridge, Cambridge, UK.
- 356 60. Rudjer Boskovic Institute, Zagreb, Croatia.
- 357 61. Department of Macromolecular Structures, Centro Nacional de Biotecnología (CNB), Consejo
358 Superior de Investigaciones Científicas (CSIC), Madrid, Spain.
- 359 62. University of Basel and ETH Zurich, 4058 Basel, Switzerland.
- 360 63. IMMM, UMR CNRS 6283, Le Mans, France.
- 361 64. School of Biosciences, University of Sheffield, Sheffield, UK.
- 362 65. Indian Institute of Science Education and Research, Pune, India.

- 363 66. i3S – Instituto de Investigação e Inovação em Saúde, Universidade do Porto, Rua Alfredo Allen
364 208, 4200-135 Porto, Portugal; INEB – Instituto de Engenharia Biomédica, Universidade do
365 Porto, Rua Alfredo Allen 208, 4200-135 Porto, Portugal; ICBAS - Instituto de Ciências
366 Biomédicas Abel Salazar da Universidade do Porto, Porto, Portugal.
- 367 67. JILA, National Institute of Standards and Technology and University of Colorado & Department
368 of Molecular, Cellular, and Developmental Biology, University of Colorado, Boulder, CO 80309,
369 USA.
- 370 68. First Department of Internal Medicine – Cardioangiology, Department of Biology, Faculty of
371 Medicine, Masaryk University, and International Clinical Research Center, St. Anne's University
372 Hospital, Brno, Czech Republic.
- 373 69. School of Sciences and Humanities, Nazarbayev University, Kazakhstan.
- 374 70. IRIM (Institut de Recherche en Infectiologie de Montpellier), Univ of Montpellier, CNRS UMR
375 9004, Montpellier, France.
- 376 71. Department of Physics “Aldo Pontremoli”, University of Milan, Milan, Italy.
- 377 72. Nano Structuring and Bio-Analytics, University of Applied Sciences Upper Austria, Austria.
- 378 73. CEITEC MU, Masaryk University, Kamenice 5, CZ-62500, Brno, Czech Republic.
- 379 74. Asylum Research - Oxford Instruments, Santa Barbara, CA, 93117 USA.
- 380 75. Aix-Marseille Université, CNRS, Inserm, Laboratoire Adhésion et Inflammation (LAI), Turing
381 centre for living systems (Centuri) , Marseille, France.
- 382 76. School of Chemical, Materials and Biological Engineering, University of Sheffield, Sheffield, UK.
- 383 77. Institute of Biophysics, University of Bremen, Germany.
- 384 78. Moleculaire Biofysica, Zernike Instituut, Rijksuniversiteit Groningen, Netherlands.
- 385 79. Department of Physics and Center for Biological Physics, Arizona State University, USA.
- 386 80. European Molecular Biology Laboratory, European Bioinformatics Institute, EMBL-EBI,
387 Cambridge, UK.
- 388 81. Institute of Applied Physics, University of Tübingen, Germany.
- 389 82. Institute of Physiology 2, University Münster, Germany.
- 390 83. School of Biomedical Engineering, Shanghai Jiao Tong University, China.
- 391 84. Laboratoire Hypoxie et Poumon, Université Sorbonne Paris Nord, Bobigny, France.
- 392 85. Department of Physics, Chemistry and Pharmacy, University of Southern Denmark (SDU), 5230
393 Odense M, Denmark.
- 394 86. Department of Mechanical Engineering, Tufts University, 200 College Ave., Medford, MA
395 02155, USA
- 396 87. i3S – Instituto de Investigação e Inovação em Saúde, Universidade do Porto, Rua Alfredo Allen
397 208, 4200-135 Porto, Portugal; INEB – Instituto de Engenharia Biomédica, Universidade do
398 Porto, Rua Alfredo Allen 208, 4200-135 Porto, Portugal; ISEP – Instituto Superior de Engenharia
399 do Porto, Instituto Politécnico do Porto, Rua Dr. António Bernardino de Almeida 431, 4249-
400 015 Porto, Portugal.
- 401 88. Biophysics and Medical Technology, Dept of Physics, The Norwegian University of Science and
402 Technology, NTNU, Trondheim, Norway.
- 403 89. School of Sciences, European University Cyprus, 6, Diogenes 2404 Engomi, Nicosia, Cyprus.
- 404 90. Faculty of Physics, Astronomy, and Computer Science, M. Smoluchowski Institute of Physics,
405 Jagiellonian University, Krakow, Poland.
- 406 91. RIKEN Center for Computational Science, Kobe, Hyogo 650-0047, Japan and Department of
407 Physics, Graduate School of Science and Institute of Transformative Bio-Molecules, Nagoya
408 University, Nagoya, Aichi 464-8601, Japan.
- 409 92. School of Dentistry and School of Physics and Astronomy, University of Leeds, Leeds, UK.
- 410 93. Physics Department, Nagoya University, Japan.
- 411 94. James Watt School of Engineering, University of Glasgow, UK.
- 412 95. Institut de Physique de Rennes, Université de Rennes, Rennes, France.
- 413 96. Laboratory of Biosensors and Bioelectronics, ETH Zurich, Zurich, CH.
- 414 97. Laboratorium für Organische Chemie, ETH Zürich, CH-8093 Zürich, Switzerland.

415 98. School of Chemistry and Chemical Engineering, Nanjing University, China.

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