PRIVATE COMPANIES LIMITED BY GUARANTEE

ARTICLES OF QUANTUM ESPRESSO FOUNDATION

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PART 1

INTERPRETATION AND LIMITATION OF LIABILITY

Defined terms

1. In the articles, unless the context requires otherwise—

"articles" means the company's articles of association;

"bankruptcy" includes individual insolvency proceedings in a jurisdiction other

than England and Wales or Northern Ireland which have an effect similar to that

of bankruptcy;

"chairman" has the meaning given in article 12;

"chairman of the meeting" has the meaning given in article 25;

"Companies Acts" means the Companies Acts (as defined in section 2 of the Companies Act 2006), in so far as they apply to the company;

"director" means a director of the company, and includes any person occupying the position of director, by whatever name called;

"document" includes, unless otherwise specified, any document sent or supplied in electronic form;

"electronic form" has the meaning given in section 1168 of the Companies Act 2006;

"member" has the meaning given in section 112 of the Companies Act 2006;

"ordinary resolution" has the meaning given in section 282 of the Companies Act 2006;

"participate", in relation to a directors' meeting, has the meaning given in article 10;

"proxy notice" has the meaning given in article 31;

"special resolution" has the meaning given in section 283 of the Companies Act 2006;

"subsidiary" has the meaning given in section 1159 of the Companies Act 2006; and

"writing" means the representation or reproduction of words, symbols or other

information in a visible form by any method or combination of methods, whether

sent or supplied in electronic form or otherwise.

Unless the context otherwise requires, other words or expressions contained in these articles bear the same meaning as in the Companies Act 2006 as in force on the date when these articles become binding on the company.

Liability of members

2. The liability of each member is limited to $\pounds 1$, being the amount that each member undertakes to contribute to the assets of the company in the event of its being wound up while he is a member or within one year after he ceases to be a member, for—

(a) payment of the company's debts and liabilities contracted before he ceases to be a member,

(b) payment of the costs, charges and expenses of winding up, and

(c) adjustment of the rights of the contributories among themselves.

PART 2

DIRECTORS

DIRECTORS' POWERS AND RESPONSIBILITIES

Directors' general authority

3.—Subject to the articles, the directors are responsible for the management of the company's business, for which purpose they may exercise all the powers of the company.

Members' reserve power

4.—(1) The members may, by special resolution, direct the directors to take, or refrain from taking, specified action.

(2) No such special resolution invalidates anything which the directors have done before the passing of the resolution.

Directors may delegate

5.—(1) Subject to the articles, the directors may delegate any of the powers which are conferred on them under the articles—

- (a) to such person or committee;
- (b) by such means (including by power of attorney);
- (c) to such an extent;
- (d) in relation to such matters or territories; and
- (e) on such terms and conditions;

as they think fit.

(2) If the directors so specify, any such delegation may authorize further delegation of the directors' powers by any person to whom they are delegated.

(3) The directors may revoke any delegation in whole or part, or alter its terms and conditions.

Committees

6.—(1) Committees to which the directors delegate any of their powers must follow procedures which are based as far as they are applicable on those provisions of the articles which govern the taking of decisions by directors.

(2) The directors may make rules of procedure for all or any committees, which prevail over rules derived from the articles if they are not consistent with them.

DECISION-MAKING BY DIRECTORS

Directors to take decisions collectively

7.—(1) The general rule about decision-making by directors is that any decision of the directors must be either a majority decision at a meeting or a decision taken in accordance with article 8.

(2) If—

(a) the company only has one director, and

(b) no provision of the articles requires it to have more than one director, the general rule does not apply, and the director may take decisions without regard to any of the provisions of the articles relating to directors' decision-making.

Unanimous decisions

8.—(1) A decision of the directors is taken in accordance with this article when all eligible directors indicate to each other by any means that they share a common view on a matter.

(2) Such a decision may take the form of a resolution in writing, copies of which have been signed by each eligible director or to which each eligible director has otherwise indicated agreement in writing.

(3) References in this article to eligible directors are to directors who would have been entitled to vote on the matter had it been proposed as a resolution at a directors' meeting.

(4) A decision may not be taken in accordance with this article if the eligible directors would not have formed a quorum at such a meeting.

Calling a directors' meeting

9.—(1) Any director may call a directors' meeting by giving notice of the meeting to the

directors or by authorising the company secretary (if any) to give such notice.

(2) Notice of any directors' meeting must indicate—

(a) its proposed date and time;

(b) where it is to take place; and

(c) if it is anticipated that directors participating in the meeting will not be in the same place, how it is proposed that they should communicate with each other during the meeting.

(3) Notice of a directors' meeting must be given to each director, but need not be in writing.

(4) Notice of a directors' meeting need not be given to directors who waive their entitlement to notice of that meeting, by giving notice to that effect to the company not more than 7 days after the date on which the meeting is held. Where such notice is given after the meeting has been held, that does not affect the validity of the meeting, or of any business conducted at it.

Participation in directors' meetings

10.—(1) Subject to the articles, directors participate in a directors' meeting, or part of a

directors' meeting, when-

(a) the meeting has been called and takes place in accordance with the articles, and

(b) they can each communicate to the others any information or opinions they have on any particular item of the business of the meeting.

(2) In determining whether directors are participating in a directors' meeting, it is irrelevant where any director is or how they communicate with each other.

(3) If all the directors participating in a meeting are not in the same place, they may decide that the meeting is to be treated as taking place wherever any of them is.

Quorum for directors' meetings

11.—(1) At a directors' meeting, unless a quorum is participating, no proposal is to be voted on, except a proposal to call another meeting.

(2) The quorum for directors' meetings may be fixed from time to time by a decision of the directors, but it must never be less than two, and unless otherwise fixed it is two.

(3) If the total number of directors for the time being is less than the quorum required, the

directors must not take any decision other than a decision-

(a) to appoint further directors, or

(b) to call a general meeting so as to enable the members to appoint further directors.

Chairing of directors' meetings

12.—(1) The directors may appoint a director to chair their meetings.

(2) The person so appointed for the time being is known as the chairman.

(3) The directors may terminate the chairman's appointment at any time.

(4) If the chairman is not participating in a directors' meeting within ten minutes of the time at which it was to start, the participating directors must appoint one of themselves to chair it.

Casting vote

13.—(1) If the numbers of votes for and against a proposal are equal, the chairman or other director chairing the meeting has a casting vote.

(2) But this does not apply if, in accordance with the articles, the chairman or other director is not to be counted as participating in the decision-making process for quorum or voting purposes.

Conflicts of interest

14.—(1) If a proposed decision of the directors is concerned with an actual or proposed transaction or arrangement with the company in which a director is interested, that director is not to be counted as participating in the decision-making process for quorum or voting purposes.

(2) But if paragraph (3) applies, a director who is interested in an actual or proposed transaction or arrangement with the company is to be counted as participating in the decision-making process for quorum and voting purposes.

(3) This paragraph applies when-

(a) the company by ordinary resolution disapplies the provision of the articles which would otherwise prevent a director from being counted as participating in the decision-making process;

(b) the director's interest cannot reasonably be regarded as likely to give rise to a conflict of interest; or

(c) the director's conflict of interest arises from a permitted cause.

(4) For the purposes of this article, the following are permitted causes—(a) a guarantee given, or to be given, by or to a director in respect of an obligation incurred by or on behalf of the company or any of its subsidiaries;

(b) subscription, or an agreement to subscribe, for securities of the company or any of its subsidiaries, or to underwrite, sub-underwrite, or guarantee subscription for any such securities; and

(c) arrangements pursuant to which benefits are made available to employees and directors or former employees and directors of the company or any of its subsidiaries which do not provide special benefits for directors or former directors.

(5) For the purposes of this article, references to proposed decisions and decision-making processes include any directors' meeting or part of a directors' meeting.(6) Subject to paragraph (7), if a question arises at a meeting of directors or of a committee of directors as to the right of a director to participate in the meeting (or part of the meeting) for voting or quorum purposes, the question may, before the conclusion of the meeting, be referred to the chairman whose ruling in relation to any director other than the chairman is to be final and conclusive.

(7) If any question as to the right to participate in the meeting (or part of the meeting) should arise in respect of the chairman, the question is to be decided by a decision of the directors at that meeting, for which purpose the chairman is not to be counted as participating in the meeting (or that part of the meeting) for voting or quorum purposes.

Records of decisions to be kept

15. The directors must ensure that the company keeps a record, in writing, for at least 10 years from the date of the decision recorded, of every unanimous or majority decision taken by the directors.

Directors' discretion to make further rules

16. Subject to the articles, the directors may make any rule which they think fit about how they take decisions, and about how such rules are to be recorded or communicated to directors.

APPOINTMENT OF DIRECTORS

Methods of appointing directors

17.—(1) Any person who is willing to act as a director, and is permitted by law to do so, may be appointed to be a director—

(a) by ordinary resolution, or

(b) by a decision of the directors.

(2) In any case where, as a result of death, the company has no members and no directors, the personal representatives of the last member to have died have the right, by notice in writing, to appoint a person to be a director.

(3) For the purposes of paragraph (2), where 2 or more members die in circumstances rendering it uncertain who was the last to die, a younger member is deemed to have survived an older member.

Termination of director's appointment

18. A person ceases to be a director as soon as—

(a) that person ceases to be a director by virtue of any provision of the Companies Act 2006 or is prohibited from being a director by law;

(b) a bankruptcy order is made against that person;

(c) a composition is made with that person's creditors generally in satisfaction of that person's debts;

(d) a registered medical practitioner who is treating that person gives a written opinion to the company stating that that person has become physically or mentally incapable of acting as a director and may remain so for more than three months;

(e) by reason of that person's mental health, a court makes an order which wholly or partly prevents that person from personally exercising any powers or rights which that person would otherwise have;

(f) notification is received by the company from the director that the director is resigning from office, and such resignation has taken effect in accordance with its terms.

Directors' remuneration

19.

(1) Directors may undertake any services for the company that the directors decide.

(2) Directors are entitled to such remuneration as the directors determine-

(a) for their services to the company as directors, and

(b) for any other service which they undertake for the company.

(3) Subject to the articles, a director's remuneration may—

(a) take any form, and

(b) include any arrangements in connection with the payment of a pension,

allowance or gratuity, or any death, sickness or disability benefits, to or in respect of that director.

(4) Unless the directors decide otherwise, directors' remuneration accrues from day to day.

(5) Unless the directors decide otherwise, directors are not accountable to the company for any remuneration which they receive as directors or other officers or employees of the company's subsidiaries or of any other body corporate in which the company is interested.

Directors' expenses

20. The company may pay any reasonable expenses which the directors properly incur in connection with their attendance at—

(a) meetings of directors or committees of directors,

(b) general meetings, or

(c) separate meetings of the holders of debentures of the company, or otherwise in connection with the exercise of their powers and the discharge of their responsibilities in relation to the company.

PART 3

MEMBERS

BECOMING AND CEASING TO BE A MEMBER

Applications for membership

21. (1) In order to be eligible to become a member, a natural or legal person must be committed to the stated objects of the Quantum ESPRESSO Foundation, agree with the company rules in force at the time, and commit to comply with them once he/she/it has become a member.

(2) No person shall become a member of the company unless—

(a) that person has completed an application for membership in a form approved

by the directors, and

(b) the directors have approved the application.

Termination of membership

22.—(1) A member may withdraw from membership of the company by giving 7 days' notice to the company in writing.

(2) Membership is not transferable.

(3) A person's membership terminates when that person dies or ceases to exist.

ORGANISATION OF GENERAL MEETINGS

Attendance and speaking at general meetings

23.—(1) A person is able to exercise the right to speak at a general meeting when that person is in a position to communicate to all those attending the meeting, during the meeting, any information or opinions which that person has on the business of the meeting.

(2) A person is able to exercise the right to vote at a general meeting when—

(a) that person is able to vote, during the meeting, on resolutions put to the vote at the meeting, and

(b) that person's vote can be taken into account in determining whether or not such resolutions are passed at the same time as the votes of all the other persons attending the meeting.

(3) The directors may make whatever arrangements they consider appropriate to enable those attending a general meeting to exercise their rights to speak or vote at it.(4) In determining attendance at a general meeting, it is immaterial whether any two or more members attending it are in the same place as each other.

(5) Two or more persons who are not in the same place as each other attend a general meeting if their circumstances are such that if they have (or were to have) rights to speak and vote at that meeting, they are (or would be) able to exercise them.

Quorum for general meetings

24. No business other than the appointment of the chairman of the meeting is to be transacted at a general meeting if the persons attending it do not constitute a quorum.

Chairing general meetings

25.—(1) If the directors have appointed a chairman, the chairman shall chair general meetings if present and willing to do so.

(2) If the directors have not appointed a chairman, or if the chairman is unwilling to chair the meeting or is not present within ten minutes of the time at which a meeting was due to start—

(a) the directors present, or

(b) (if no directors are present), the meeting, must appoint a director or member to chair the meeting, and the appointment of the chairman of the meeting must be the first business of the meeting.

(3) The person chairing a meeting in accordance with this article is referred to as "the chairman of the meeting".

Attendance and speaking by directors and non-members

26.—(1) Directors may attend and speak at general meetings, whether or not they are members.

(2) The chairman of the meeting may permit other persons who are not members of the company to attend and speak at a general meeting.

Adjournment

27.—(1) If the persons attending a general meeting within half an hour of the time at which the meeting was due to start do not constitute a quorum, or if during a meeting a quorum ceases to be present, the chairman of the meeting must adjourn it.

(2) The chairman of the meeting may adjourn a general meeting at which a quorum is present if—

(a) the meeting consents to an adjournment, or

(b) it appears to the chairman of the meeting that an adjournment is necessary to protect the safety of any person attending the meeting or ensure that the business of the meeting is conducted in an orderly manner.

(3) The chairman of the meeting must adjourn a general meeting if directed to do so by the meeting.

(4) When adjourning a general meeting, the chairman of the meeting must-

(a) either specify the time and place to which it is adjourned or state that it is to continue at a time and place to be fixed by the directors, and

(b) have regard to any directions as to the time and place of any adjournment which have been given by the meeting.

(5) If the continuation of an adjourned meeting is to take place more than 14 days after it was adjourned, the company must give at least 7 clear days' notice of it (that is, excluding the day of the adjourned meeting and the day on which the notice is given)—

(a) to the same persons to whom notice of the company's general meetings is required to be given, and

(b) containing the same information which such notice is required to contain.(6) No business may be transacted at an adjourned general meeting which could not properly have been transacted at the meeting if the adjournment had not taken place.

VOTING AT GENERAL MEETINGS

Voting: general

28. A resolution put to the vote of a general meeting must be decided on a show of hands unless a poll is duly demanded in accordance with the articles.

Errors and disputes

29.—(1) No objection may be raised to the qualification of any person voting at a general meeting except at the meeting or adjourned meeting at which the vote objected to is tendered, and every vote not disallowed at the meeting is valid. (2) Any such objection must be referred to the chairman of the meeting whose decision is final.

Poll votes

30.—(1) A poll on a resolution may be demanded—

(a) in advance of the general meeting where it is to be put to the vote, or

(b) at a general meeting, either before a show of hands on that resolution or

immediately after the result of a show of hands on that resolution is declared.

(2) A poll may be demanded by—

(a) the chairman of the meeting;

(b) the directors;

(c) two or more persons having the right to vote on the resolution; or

(d) a person or persons representing not less than one tenth of the total voting rights of all the members having the right to vote on the resolution.

(3) A demand for a poll may be withdrawn if—

(a) the poll has not yet been taken, and

(b) the chairman of the meeting consents to the withdrawal.

(4) Polls must be taken immediately and in such manner as the chairman of the meeting directs.

Content of proxy notices

31.—(1) Proxies may only validly be appointed by a notice in writing (a "proxy notice") which—

(a) states the name and address of the member appointing the proxy;

(b) identifies the person appointed to be that member's proxy and the general meeting in relation to which that person is appointed;

(c) is signed by or on behalf of the member appointing the proxy, or is authenticated in such manner as the directors may determine; and

(d) is delivered to the company in accordance with the articles and any

instructions contained in the notice of the general meeting to which they relate.

(2) The company may require proxy notices to be delivered in a particular form, and may specify different forms for different purposes.

(3) Proxy notices may specify how the proxy appointed under them is to vote (or that the proxy is to abstain from voting) on one or more resolutions.

(4) Unless a proxy notice indicates otherwise, it must be treated as-

(a) allowing the person appointed under it as a proxy discretion as to how to vote on any ancillary or procedural resolutions put to the meeting, and

(b) appointing that person as a proxy in relation to any adjournment of the general meeting to which it relates as well as the meeting itself.

Delivery of proxy notices

32.—(1) A person who is entitled to attend, speak or vote (either on a show of hands or on a poll) at a general meeting remains so entitled in respect of that meeting or any adjournment of it, even though a valid proxy notice has been delivered to the company by or on behalf of that person.

(2) An appointment under a proxy notice may be revoked by delivering to the company a notice in writing given by or on behalf of the person by whom or on whose behalf the proxy notice was given.

(3) A notice revoking a proxy appointment only takes effect if it is delivered before the start of the meeting or adjourned meeting to which it relates.

(4) If a proxy notice is not executed by the person appointing the proxy, it must be accompanied by written evidence of the authority of the person who executed it to execute it on the appointor's behalf.

Amendments to resolutions

33.—(1) An ordinary resolution to be proposed at a general meeting may be amended by ordinary resolution if—

(a) notice of the proposed amendment is given to the company in writing by a person entitled to vote at the general meeting at which it is to be proposed not less than 48 hours before the meeting is to take place (or such later time as the chairman of the meeting may determine), and

(b) the proposed amendment does not, in the reasonable opinion of the chairman of the meeting, materially alter the scope of the resolution.

(2) A special resolution to be proposed at a general meeting may be amended by ordinary resolution, if—

(a) the chairman of the meeting proposes the amendment at the general meeting at which the resolution is to be proposed, and

(b) the amendment does not go beyond what is necessary to correct a

grammatical or other non-substantive error in the resolution.

(3) If the chairman of the meeting, acting in good faith, wrongly decides that an amendment to a resolution is out of order, the chairman's error does not invalidate the vote on that resolution.

PART 4

ADMINISTRATIVE ARRANGEMENTS

Means of communication to be used

34.—(1) Subject to the articles, anything sent or supplied by or to the company under the articles may be sent or supplied in any way in which the Companies Act 2006 provides for documents or information which are authorised or required by any provision of that Act to be sent or supplied by or to the company.

(2) Subject to the articles, any notice or document to be sent or supplied to a director in connection with the taking of decisions by directors may also be sent or supplied by the means by which that director has asked to be sent or supplied with such notices or documents for the time being. (3) A director may agree with the company that notices or documents sent to that director in a particular way are to be deemed to have been received within a specified time of their being sent, and for the specified time to be less than 48 hours.

Company seals

35.—(1) Any common seal may only be used by the authority of the directors.

(2) The directors may decide by what means and in what form any common seal is to be used.

(3) Unless otherwise decided by the directors, if the company has a common seal and it is affixed to a document, the document must also be signed by at least one authorised person in the presence of a witness who attests the signature.

(4) For the purposes of this article, an authorised person is—

(a) any director of the company;

(b) the company secretary (if any); or

(c) any person authorised by the directors for the purpose of signing documents to which the common seal is applied.

No right to inspect accounts and other records

36. Except as provided by law or authorised by the directors or an ordinary resolution of the company, no person is entitled to inspect any of the company's accounting or other records or documents merely by virtue of being a member.

Provision for employees on cessation of business

37. The directors may decide to make provision for the benefit of persons employed or formerly employed by the company or any of its subsidiaries (other than a director or former director or shadow director) in connection with the cessation or transfer to any person of the whole or part of the undertaking of the company or that subsidiary.

DIRECTORS' INDEMNITY AND INSURANCE

Indemnity

38.—(1) Subject to paragraph (2), a relevant director of the company or an associated company may be indemnified out of the company's assets against—

(a) any liability incurred by that director in connection with any negligence, default, breach of duty or breach of trust in relation to the company or an associated company,

(b) any liability incurred by that director in connection with the activities of the company or an associated company in its capacity as a trustee of an occupational pension scheme (as defined in section 235(6) of the Companies Act 2006),

(c) any other liability incurred by that director as an officer of the company or an associated company.

(2) This article does not authorise any indemnity which would be prohibited or rendered void by any provision of the Companies Acts or by any other provision of law.

(3) In this article—

(a) companies are associated if one is a subsidiary of the other or both are subsidiaries of the same body corporate, and

(b) a "relevant director" means any director or former director of the company or an associated company.

Insurance

39.—(1) The directors may decide to purchase and maintain insurance, at the expense of the company, for the benefit of any relevant director in respect of any relevant loss. (2) In this article—

(a) a "relevant director" means any director or former director of the company or an associated company,

(b) a "relevant loss" means any loss or liability which has been or may be incurred by a relevant director in connection with that director's duties or powers in relation to the company, any associated company or any pension fund or employees' share scheme of the company or associated company, and(c) companies are associated if one is a subsidiary of the other or both are subsidiaries of the same body corporate.

PART 5

OBJECTS AND PROFIT POLICY

Objects

40. The object of the company is to foster and support cooperation in the development, design, implementation, maintenance, and free dissemination of high-quality, high-performance open-source scientific software for the *ab-initio* quantum numerical modeling of materials. This object will be pursued by:

- a. coordinating and supporting research within the *Quantum ESPRESSO* developers community, aimed at enhancing the scope and performance of the *Quantum ESPRESSO* software;
- b. supporting the growth of the *Quantum ESPRESSO* users and developers communities;
- c. holding and administering the copyright of the *Quantum ESPRESSO* software and documentation, and protecting its open-source character and free distribution;
- d. promoting education and advanced training in the field of the quantum simulation of materials, by organizing or sponsoring courses, conferences, and workshops based on the use of the *Quantum ESPRESSO* software worldwide, with particular emphasis on developing countries
- e. acting as the official voice of the *Quantum ESPRESSO* project. The company will represent its users and developers community at scientific meetings. It will also provide means of communication with the press, and with academic, as well as non academic, and non commercial, as well as commercial, organizations interested in the *Quantum ESPRESSO* project and software.

Non-profit making

(1) The company's income shall be applied only in promoting its objects, as stated above.

(2) The company shall not pay dividends or make any return of capital to its members.