

QUANTUM THEORY PROJECT

Original Charter February 25, 1987

Revised Charter, April 8, 2004

Endorsed by QTP Faculty secret ballot, April 16, 2004

Minor revisions, July 1, 2004, as recommended by the College of Liberal Arts and Sciences

Revised Charter, October 8, 2007

Revised Charter, January 11, 2011

Endorsed by QTP Faculty secret ballot, January 21, 2011

Revised Charter, May 7, 2019

Endorsed by QTP Faculty secret ballot, May 15, 2019

I. Change Record

1. The Quantum Theory Project (QTP) began in 1960. At that time the University of Florida had no official framework for Centers and Institutes.
2. In 1987, QTP became the “Institute for Theory and Computation in Molecular and Materials Sciences”, a Type II Center in the State University System of Florida. The Proposal for that reorganization (Jan. 15, 1987) became the Charter under which the Institute operated.
3. In 2001, the State University System was restructured. The charter was revised in 2004 to
 - a. remove anachronistic detail without altering basic governance, reporting, and financial structures;
 - b. modify the Charter to reflect actual practice the Institute had found useful since 1987.
4. In April 2007, the request to change the official name of the Institute back to the known name “Quantum Theory Project” was approved.
5. In Oct 2007, the Charter was revised and updated with the following amendments:
 - a. Section IV.A: abolish the elected position of Supervisor of the John C. Slater Laboratory;
 - b. Section V.B: update the resource list;
 - c. Appendix B: Update the member lists.
6. In Jan 2011, the Charter was updated to reflect changes in status of the members and in resources (Section V.B). It was amended (Section II.A and Section III.A) to remove the restriction that members of QTP must be members of the Department of Chemistry or Physics. The description of the election for Director and Associate Director was (Section IV.A.iv) was amended from two-thirds majority to simple majority.
7. In May 2019, the Charter was updated to clarify the roles of three types of faculty members and the procedure for becoming QTP Faculty members.

II. Type and Purpose

A. Type and Name

The Quantum Theory Project is a Type II Center (or such equivalent category as may subsequently be established by the University of Florida and/or the State University System or its successor) in the

College of Liberal Arts and Sciences and College of Engineering. It is known informally by the abbreviation QTP. For simplicity that name is used in this document.

B. Purpose

The primary purpose of the QTP is to provide a framework to draw together faculty with, interdisciplinary research interests in the theory of the structure and dynamics of matter in the gas phase, the condensed phase, and in biological systems, as well as applications of theory to predicting and understanding processes and properties of molecules, materials, and biological systems. QTP's corollary purposes are to facilitate and coordinate the advance of research, instruction, and public understanding in related areas of the mathematical and computational sciences in which the QTP members have expertise. Thus, QTP shall foster both individual effort and close collaborations in these areas of research and education, and in seeking extramural funding for them. It shall recruit high-quality graduate students, postdoctoral associates, and undergraduate students. QTP may offer specialized courses within the departments from which QTP faculty are drawn, and may, upon receipt of appropriate authorizations, offer courses, certificates, and degrees in its own right or in conjunction with those departments. It shall organize international scientific meetings, exemplified by the long-standing Sanibel Symposium series, as well as workshops and short courses. QTP has a long tradition of fostering a stimulating scientific and professional cross-cultural environment, an important feature that we plan to maintain.

III. Membership

Types of membership are defined as follows:

A. Regular Faculty Member

A person may become a QTP Regular Faculty Member if she or he is a faculty member at the University of Florida (Asst. Prof., Assoc. Prof., Prof., Distinguished Prof., Named Prof., Emeritus Prof., Asst. Scientist, Assoc. Scientist, or Scientist), commits to contributing to QTP and participating in QTP activities, and is approved by a three-quarters majority vote of the regular members at the time of the decision. Contribution to QTP is made through returned overhead and/or in-kind. Regular Faculty Members have full voting rights and may run for positions as QTP officers subject to eligibility requirements. If a Regular Faculty Member fails to contribute to QTP, the membership may be terminated upon a majority vote of Regular Faculty Members. Regular without current funding are excused from contributions. Regular Faculty Membership is automatically terminated if the faculty leaves the University of Florida.

B. Emeritus Member

A Regular Faculty Member becomes an Emeritus Member by virtue of reaching Emeritus status in his/her home Department and ceasing to contribute to QTP. Emeritus Members have the right to participate in all aspects of QTP's activities (including faculty meetings) and to vote on all topics except for personnel matters and resource allocation matters. An Emeritus Member who meets all requirements of a Regular Faculty Member may be reinstated as a Regular Member upon a majority vote of Regular Faculty members.

C. Affiliate Member

A modest number of persons may become Affiliate Members if they meet the criteria listed in Appendix A. Affiliate Faculty do not participate in QTP Faculty meetings (except if invited as guests by vote of the regular faculty). The term of service is five years, renewable by mutual consent. QTP may terminate the relationship, by action of the QTP Regular Faculty. The process for conferring or renewing this status to be used by the QTP regular faculty is: (i) For initial appointment, evaluation of the fitness of the nominee according to the criteria listed in Appendix A; (ii) For renewal appointment, evaluation of

the specific contributions to the QTP (during the period ending) by visits, collaborations, and other activities that demonstrate results consistent with the criteria listed in Appendix A. Secret ballot of the Regular Faculty with a simple majority vote in favor is required both for appointment and renewal as an affiliate member.

E. General Membership

All other persons (undergraduate research students, graduate research students, postdoctoral associates, senior professional staff, administrative and clerical staff) who are resident in the Institute and are not guests by the nature of their stay, are Members for the duration of their appointed involvement (paid or approved volunteer) with QTP.

F. Faculty Membership List

A list of Regular, Emeritus, Affiliate faculty members shall be maintained by QTP and updated ~~at least~~ annually. The Faculty membership list is not a part of this Charter, but for the record, the version of the list as of the date that QTP faculty voted upon adoption or revision of this Charter is given in Appendix B.

IV. Governance

A. Officers

QTP shall have the following officers, terms of office, and method of election.

- i. *Director.* The Director shall have been an Institute regular faculty member for at least two academic years prior to beginning service. A person may not serve more than three consecutive terms as Director.
- ii. *Associate Director.* The Associate Director shall be an Institute regular faculty member who is eligible to serve as Director. There is no limit on consecutive terms of service as Associate Director. The Associate Director shall serve as Acting Director in the Director's absence or at the Director's request, and shall fulfill such other administrative and leadership roles for the Institute as the Director may request.
- iii. *Finance officer.* The Finance Officer shall be an Institute regular faculty member. There is no limit on consecutive terms of service as Finance Officer. The Finance Officer oversees expense disbursement and reports annually all contributions to the QTP.
- iv. The leadership of QTP, as defined by Director, Associate Director and Finance Officer, must be drawn from at least two different departments.
- v. The terms of the two offices (Director, Assoc. Director) shall be three years, from 1 January of the first year through 31 December of the third.
- vi. The election for the Director and the Associate Director shall be held no later than 1 November in the year in which the three-year terms end, and shall be conducted by secret ballot of the regular faculty. (Elections in Fall 2020, Fall 2023, Fall 2026, etc.) A simple majority of the eligible faculty shall prevail for each of the two offices.

B. Absences

When both the Director and Associate Director are to be absent, the Director may designate any member of the regular faculty to be Acting Director for a stated period.

C. Policy Adoptions

Within the bounds of this Charter and the applicable regulations and policies of the University, authority for adopting general policies for the Institute shall reside with the regular faculty members of the Institute plus those Emeriti, and or Affiliates who have specific voting rights as delineated above. The

Director shall assure that there is at least one meeting of the Faculty per semester. If at least one-third (1/3) of the regular Faculty Members request a meeting to consider a specific topic or proposal, the Director shall convene such a meeting promptly.

D. Annual Review

The Director (with the cooperation of the Assoc. Director) shall prepare an Annual Program Review for the Deans of the College of Liberal Arts and Sciences and the College of Engineering. On substantive matters of policy and administration, the Director shall consult with the Chairs of the departments of all faculty members and shall report to the Dean of relevant colleges.

E. Information Sharing

For the purposes of coordination and information sharing, the Director shall meet at least annually with the Provost and with the Vice President for Research.

V. Resources

A. Primary Fiscal Resources

The primary fiscal resources for the research efforts of QTP Faculty Members consist of their research grants and contracts with federal agencies and/or private industry.

B. University Fiscal Resources

University fiscal resources for other QTP activities shall consist primarily of those listed below.

- i. Staff members are supervised by the Director and provide primarily support for the members of QTP;
- ii. Returned indirect cost funds, grants, and contracts designated to QTP.
- iii. The Institute also may have a variety of Foundation funds, including those in existence at the time of adoption of this charter.

D. Human Resources

Permanent staff positions are assigned by the College of Liberal Arts and Sciences and the College of Engineering. Staff report to the Director or the Director's designee.

VI. Voting

A. Majority requirements for various kinds of membership and for the officers of QTP are stipulated in the corresponding subsections of this Charter.

B. Adoption and any subsequent amendment of this Charter requires a secret ballot and at least a three-quarters ($\frac{3}{4}$) majority of the QTP Regular Faculty.

C. Any matter not requiring secret ballot will be decided by simple majority vote of the eligible faculty present when the matter is proposed. Written proxies for a specific matter that will come up for voice vote may be used by a faculty member who must be absent.

D. Voting is administered by a Regular Faculty Member designated by the Director. The form of voting is determined by the Director.

Appendix A. Eligibility Criteria for Affiliate Faculty

The basic criteria for consideration of conferring Affiliate Faculty status on a person include the following: (i) Significant research achievements in one or more of the fields of main relevance to QTP; (ii) A collaboration with at least one member of the QTP's regular faculty prior to assuming the role; (iii) Demonstrated, supportive interest in the research program of QTP; (iv) Capability and willingness for making meaningful contributions to the scientific work of QTP on a continuing basis; (v) Acceptance (either prior or concurrent) of the person as an Adjunct Faculty member by the Univ. Florida. Other criteria may be stipulated at the time the status is conferred or renewed.

Appendix B. Faculty Member List

Remark: This list *per se* is not a part of the charter but is provided for convenience and for historical record as of the date the charter was submitted to QTP faculty for adoption.

As of September 4, 2018:

Faculty Members

- Rodney J. Bartlett (Graduate Research Professor, Chemistry and Physics)
- Hai-Ping Cheng (Professor, Physics)
- Erik Deumens (Scientist, Chemistry and Physics)
- Frank Harris (Research Professor, Chemistry)
- Richard G. Hennig (Professor, Materials Science and Engineering)
- Ajith Perera (Scientist, Chemistry)
- Simon R. Phillpot (Professor, Materials Science and Engineering)
- Beverly Sanders (Associate Professor, Computer & Information Science & Engineering)
- John F. Stanton (W.R. Kenan Professor, Chemistry)
- Xiaoguang Zhang (Professor, Physics)

Emeritus Faculty Members

- David A. Micha (Professor Emeritus, Chemistry and Physics)
- Hendrik J. Monkhorst (Professor Emeritus, Physics)
- N. Yngve Öhrn (Professor Emeritus, Chemistry)
- John R. Sabin (Professor Emeritus, Physics)
- Samuel B. Trickey (Professor Emeritus, Physics)

Affiliate Faculty Members

- Malcolm Stocks
- Tony Gonis

Appendix C. Previous Members

- So Hirata (Assistant Professor, Chemistry)
- Jeffrey L. Krause (Professor, Chemistry and Physics)(On leave Aug 20, 2006 – Aug 20, 2008)
- Per-Olov Löwdin (Graduate Research Professor, Chemistry and Physics)
- Kenneth M. Merz (Professor, Chemistry)
- Nigel Richards (Professor, Chemistry)
- Adrian E. Roitberg (Associate Professor, Chemistry)

- John C. Slater (Graduate Research Professor, Physics and Chemistry)
- Susan B. Sinnott (Professor, Materials Science and Engineering)
- Michael C. Zerner (Professor, Chemistry)
- Chris J. Stanton (Professor, Physics; term = 2005-2010)
- Neil Ostlund (term=2005-2010)
- Mark Ponton (term=2003-2008)
- Keith Runge (term=2005-2010)

Information from Sam Trickey:

Charles E. Reid (Prof., Chemistry)
 John W.D. Connolly (Prof., Physics)
 James B. Conklin Jr. (Prof. Physics)
 George D. Purvis (Scientist, Chemistry)
 Richard Lozes (Assoc. Scientist, Chemistry)

Before I joined QTP (01 Jan. 1969) there were

John S. Faulkner (Asst Prof. Physics; I don't know if he was promoted or not before leaving)
 Richard F. Wood (Asst. Prof. Physics; also don't know about promotion before he left)
 Darwin W. Smith (Asst. Prof., Chem.; also don't know about promotion before he left)
 Donald E. Ellis (Asst. Prof. Physics; same question about promotion)
 Timothy M. Wilson (Asst. Prof. Physics; he left after one year)