

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

Revised Charter, October 8, 2007

Revised Charter, January 11, 2011

Endorsed by QTP faculty secret ballot, January 21, 2011

I. Change Record

1. 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) conform the Charter to actual practice the Institute has 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, this document was updated to reflect changes in status of the members and in resources (Section V.B). The charter 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.

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. The Institute is known informally

by the abbreviation “QTP”. For brevity that name and “the Institute” are used interchangeably in this document.

B. Purpose

The primary purpose of the Institute is to provide a recognized framework within which to draw together faculty with strong, shared, interdisciplinary research interests in the theory of the structure and dynamics of matter in gas phase, condensed phases, and in biological systems, and in applications of the theory to predicting and understanding processes and properties of molecules, materials, and biological systems. The Institute’s corollary purposes are to facilitate and coordinate the advance of research, instruction, and public understanding in the segments of mathematical and computational sciences in which the Institute’s members have competence. Thus, the Institute shall foster both individual effort and close collaborations in these areas of research and graduate studies and in seeking extramural funding for them. It shall recruit high-quality graduate students, post-doctoral associates, and undergraduate students. It shall enable sharing of instrumentation, primarily computer and network systems in the John C. Slater Computing Laboratory. The Institute may offer specialized courses within its host departments and may, upon receipt of appropriate authorizations, offer courses, certificates, and degrees in its own right or in conjunction with its host departments. It shall organize international scientific meetings, exemplified by the long-standing Sanibel Symposium series and the Pan American Workshops on Molecular and Materials Sciences, as well as workshops and short courses.

III. Membership

Types of membership are defined as follows. The “regular faculty” consist of members in category III.A.

A. Regular Faculty

A person may become a Faculty Member of the Institute if she or he is a regular faculty member at the University of Florida (Asst. Prof., Assoc. Prof., Prof., distinguished or named Professors, Asst. Scientist, Assoc. Scientist, Scientist), and is approved by vote with a majority of at least three-quarters of the then-current regular members.

B. Emeritus Faculty

A Faculty Member becomes an Emeritus Member by virtue of reaching Emeritus status in his/her home Department. Emeritus Members have the right to participate in all aspects of QTP’s work and in QTP Faculty meetings and to vote on all topics except for personnel matters (including but not limited to recommendations to the host Departments and determination of Adjunct status) and resource allocation matters (funds and space).

C. Resident Adjunct Faculty

In occasional special cases of clear and unusual benefit to the broad program of QTP, regular faculty of the Institute may invite a person to affiliate in the status of Resident Adjunct Professor. Resident Adjunct Professors have the right to speak on all matters before the QTP regular faculty and to vote on all topics save for personnel matters (including but not

limited to recommendations to the parent Departments and determination of Adjunct status) and resource allocation matters (funds and space). The term of service is five years, renewable by mutual consent, terminable at the sole option of QTP regular faculty. The process both for conferring this status and of review for continuation in it is (i) Evaluation by QTP regular faculty of the fitness of the nominee according to the criteria listed in Appendix A; (ii) Secret ballot by regular faculty of QTP with at least 2/3rds (two-thirds) majority in favor. To continue or be renewed in this status, a person must have a solid record of actual fulfillment of both the criteria given in Appendix A and any other considerations that may have been stipulated at the time the status was conferred.

D. Adjunct Faculty and Industrial Affiliate Members

A modest number of persons may become Adjunct Members or Industrial Affiliate Members if they meet the criteria listed in Appendix A. Adjunct Faculty and Industrial Affiliates 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 at its sole option, 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 Institute (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. Adjunct Faculty are distinguished from Industrial Affiliates by the nature of their primary professional employment.

E. General Membership

All other persons (undergraduate research students, graduate research students, post-doctoral 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 the Institute.

F. Faculty Membership List

A list of Regular, Emeritus, Resident Adjunct, Adjunct, and Industrial Affiliate faculty members shall be maintained by the Institute 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 of this Charter is given in Appendix B.

IV. Governance

A. Officers

The Institute 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. The Director shall serve as administrator

- 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. 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.
- iv. The election for these two offices shall be held no later than Nov. 1 in the year in which the three-year terms end, and shall be conducted by secret ballot of the regular faculty. (Elections in Fall 1998, Fall 2001, Fall 2004, etc.) A simple majority of the eligible faculty shall prevail for each of the two offices.

B. 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. 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, Adjuncts, 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. The Director (with the cooperation of the Assoc. Director) shall prepare an Annual Program Review for the Dean of Liberal Arts and Sciences. On substantive matters of policy and administration, the Director shall consult with the Chairs of Chemistry and of Physics and shall report to the Dean of Liberal Arts and Sciences.

E. 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.

F. If resources allow, the Institute should arrange for regular (approximately every five years) outside review and evaluation of its activities by a compact panel of distinguished scientists.

V. Resources

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

B. University fiscal resources for other Institute 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 In-direct Cost funds grants and contracts designated to the Institute;
- iii. Auxiliary funds for the maintenance and operation of the J.C. Slater Computing Facility.

C. 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. The Office Manager reports to the Director. The rest of the staff report to the Office Manager unless otherwise decided by the Director.

E. Space: Adequate space for the Institute's personnel, computing facility, and other mission-driven requirements shall be assigned to the Institute by the College of Liberal Arts and Sciences via the host departments. The Institute shall manage that space to best meet its mission. (Informally arranged short-term space does not fall under this provision.)

VI. Voting

A. Majority requirements for various kinds of membership and for the officers of the Institute 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 two-thirds (2/3) majority of the regular faculty of the Institute.

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.

Appendix A. Eligibility Criteria for Resident Adjunct Faculty, Adjunct Faculty, and Industrial Affiliates

A. The basic criteria for consideration of conferring Resident Adjunct Faculty status upon a person include the following: (i) Unquestioned stature in the fields of primary interest to QTP; (ii) History of active collaborations with more than one member of the QTP regular faculty prior to assuming this role; (iii) Demonstrated interest in and capability of sustaining an active, high-quality research program relevant to the scientific work of the Institute; (iv) Demonstrated interest in and capability of contributing substantially to the scientific work of the Institute on a continuing basis; (v) Explicit commitment to being in residence at QTP a substantial fraction of each year; (vi) Explicit willingness to assume an active role in the programmatic work of QTP, including attracting new funds, organizing the Sanibel Symposia, participating in and organizing short courses, etc.; (vii) Acceptance (either prior or concurrent) of the person as an Adjunct faculty member by one or both of the parent Departments of QTP. Additional criteria may be stipulated at the time the status is conferred or renewed.

B. The basic criteria for consideration of conferring Adjunct Faculty status or Industrial Affiliate Member status on a person include the following: (i) Significant research achievements in one or more of the fields of main relevance to The Institute; (ii) A collaboration with at least one member of the Institute's regular faculty prior to assuming the role; (iii) Demonstrated, supportive interest in the research program of the Institute; (iv) Capability and willingness for making meaningful contributions to the scientific work of the Institute on a continuing basis; (v) Acceptance (either prior or concurrent) of the person as an Adjunct faculty member by the Univ. Florida Department of Chemistry or of Physics or both. 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 January 21, 2011:

Faculty Members

Rodney J. Bartlett (Graduate Research Professor, Chemistry and Physics)
Hai-Ping Cheng (Professor, Physics)
Erik Deumens (Scientist, Chemistry and Physics)
Kenneth M. Merz (Professor, Chemistry)
Nigel Richards (Professor, Chemistry)
Simon R. Phillpot (Professor, Materials Science and Engineering, pending vote)
Adrian E. Roitberg (Associate Professor, Chemistry)
John R. Sabin (Professor, Physics and Chemistry)
Susan B. Sinnott (Professor, Materials Science and Engineering, pending vote)

Emeritus Faculty Members

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

Resident Adjunct Faculty Members

Frank E. Harris (Chemistry; term = 2011 - 2015)

Adjunct Faculty Members

Chris J. Stanton (Professor, Physics; term = 2011 - 2015)

Industrial Affiliate Faculty Members

Keith Runge (term = 2011-2015)

Appendix C. Previous Faculty Member List

As of August 31, 2007:

Faculty Members

Rodney J. Bartlett (Graduate Research Professor, Chemistry and Physics)

Hai-Ping Cheng (Professor, Physics)

Erik Deumens (Scientist, Chemistry and Physics)

So Hirata (Assistant Professor, Chemistry)

Jeffrey L. Krause (Professor, Chemistry and Physics)(On leave Aug 20, 2006 – Aug 20, 2008)

Kenneth M. Merz (Professor, Chemistry)

David A. Micha (Professor, Chemistry and Physics)(until Dec 31, 2007)

Hendrik J. Monkhorst (Professor, Physics and Chemistry)

N. Yngve Öhrn (Professor, Chemistry and Physics)(until Dec 31, 2007)

Nigel Richards (Professor, Chemistry)

Adrian E. Roitberg (Associate Professor, Chemistry)

John R. Sabin (Professor, Physics and Chemistry)

Emeritus Faculty Members

David A. Micha (Professor Emeritus, Chemistry and Physics)(after Jan 1, 2008)

N. Yngve Öhrn (Professor Emeritus, Chemistry and Physics)(after Jan 1, 2008)

Samuel B. Trickey (Professor Emeritus, Physics and Chemistry)

Resident Adjunct Faculty Members

Frank E. Harris (Chemistry; term =2005 - 2010)

Adjunct Faculty Members

Chris J. Stanton (Professor, Physics; term = 2005 - 2010)

Industrial Affiliate Faculty Members

Neil Ostlund (term=2005-2010)

Mark Ponton (term=2003-2008)

Keith Runge (term=2005-2010)