

# QTP History

## Yngve Öhrn

Leigh Hall



1/31 2018

Quantum Theory Project

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# Per-Olov Löwdin

- 1960-1983 held the chair of Quantum Chemistry at Uppsala University, Sweden.
- January 1960 appointed Graduate Research Professor of Chemistry and Physics at University of Florida.
- This marks the beginning of QTP, The Quantum Theory Project for Research in Atomic, Molecular, and Solid-State Theory.

# Pioneering Scientist

- PhD (FD) 1948
- Dissertation: QM Calculation on the cohesive energy and elastic constants of Alkali Halides.
- Great effort using human multi-processor setup.
- Good results helped by fortuitous cancellation of errors.
- Clever combination of energy terms.

# POL

- Failure of the Cauchy relations for elastic constants of ionic crystals was a motivation.
- POL showed that many-atom interactions should be considered beyond the “classical” two-body potentials.
- The additional terms come from overlap integrals among atomic orbitals

# POL CONCEPTS

- CORRELATION ENERGY
- NATURAL ORBITALS, CI CONVERGENCE
- REDUCED DENSITY MATRICES
- “SYMMETRY DILEMMA”
- GROUP ALGEBRA
- NON-ORTHOGONALITY AND LINEAR DEPENDENCE



# Faculty associated with early QTP

- Samuel Faulkner, Physics
- Richard Wood, Physics
- Darwin Smith, Chemistry
- Charles Reid, Chemistry
- Visitors:
  - Jan Linderberg, Jean-Louis Calais, Klaus Appel, Jan Nordling, Yngve Öhrn, Egil Hylleraas, Ludwig Hofacker, Werner Bingel, Joseph Hirschfelder, Kimio Ohno, Ruben Pauncz, Manfred Eigen, etc. etc.

# John C Slater

Head of the Department of Physics at MIT,  
joined QTP in 1964.

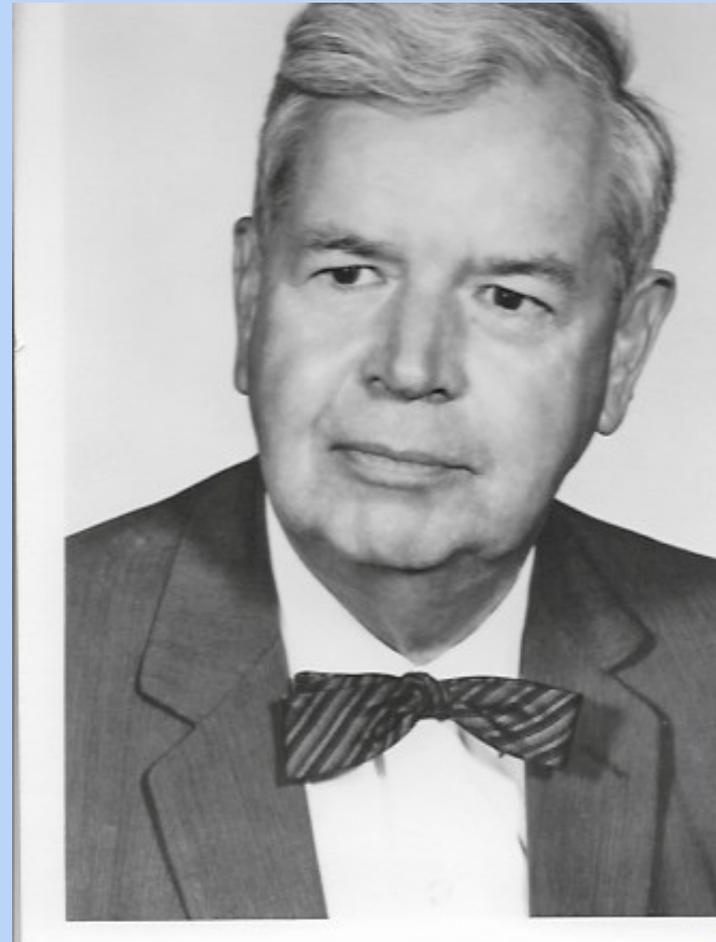
Some came and went:

James Conklin, Donald Ellis, Timothy Wilson,  
John Connolly [Student, Later UF Faculty]

Some came and stayed:

Samuel B Trickey, David Micha, John R Sabin,  
Hendrick J Monkhorst

# POL:Equations; JCS: Words



# JCS'S SCIENCE

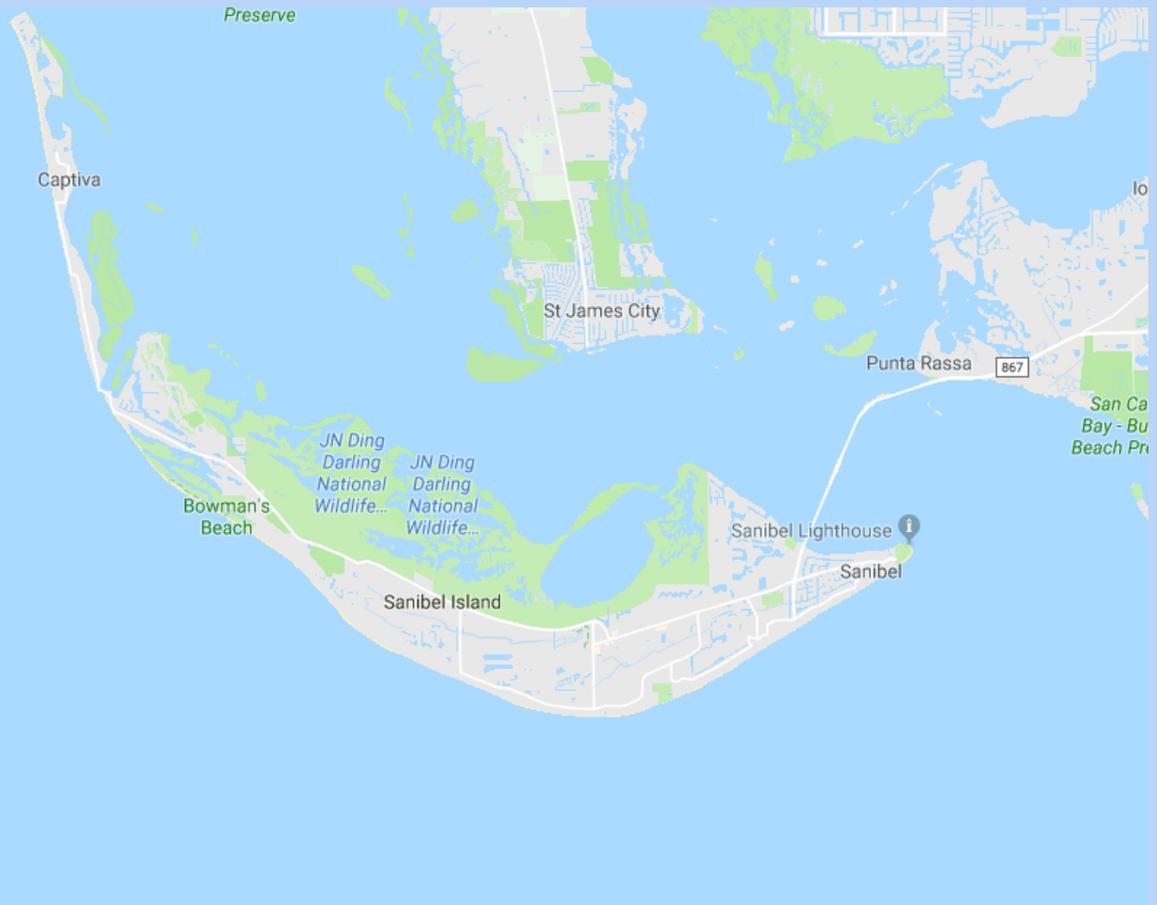
- ATOMIC CENTRAL FIELD MODEL
- SPIN ORBITALS, DETERMINANTAL WF
- SLATER ORBITALS
- X-ALPHA
- NUMEROUS BOOKS
- 1976 NOBEL PRIZE COULD HAVE BEEN HIS

# Educational Efforts

- The Uppsala Scandinavian Summer Schools (1958-1987) in Quantum Chemistry were duplicated in Florida with similar Winter programs.
- About 15 of these schools were held in the 1970's and 1980's., combined with Sanibel Symp.
- The annual Sanibel Symposia started around New year 60/61 first on Sanibel Island, and later at Palmcoast Sheraton, Marineland, and Ponce de Leon conference center, St Augustine, FL., and lately at the King&Prince St Simons Island.

# QTP Students in Norway 1976





# Attentive students at 1963 Sanibel



# Klaus, Alex, and Joe on break



# Major expansion of QTP

In 1982 the arrival of Rodney J. Bartlett and Michael C. Zerner added people, talent, and resources to QTP.

The computing support improved with the arrival of George D. Purvis.

Bartlett led a successful Molecular Orbital School for a few years designed for industry: Bartlett, Zerner, Dewar, and Öhrn lectured and Purvis led the applications part.

# Students

- PhD's from QTP hold leadnig positions in Industry, Government, and Academe in the USA, Europe, South America, and Asia.

Including the hundreds of Postdoctoral Associates of QTP the list of QTP alumni in elevated positions around the world becomes even more impressive.

# 2000 and beyond

- Expansion of QTP beyond the founding departments of Physics and Chemistry by researchers from Material Science,
- Richard Henning, Simon Phillipot
- and Computer Science,
- Beverly Sanders
- Going from Residential to Paper Institute.

# Informal Assoc. to Institute

- From its start in 1960 and for the next 27 years QTP was an informal association of Physics and Chemistry faculty and their research groups occupying contiguous space in Leigh Hall and later in the Nuclear Science Building, and even later in Williamson Hall, and eventually NPB.
- In 1987 QTP became a formal Type II Institute with a budget and a formal presence at UF.



QTP 2007?

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# Late 1980's-Present

- Some came and went: Jeffrey Krause, Kenneth Mertz, So Hirata, Nigel Richards, Adrian Roitberg
- Some came and stayed: H-P Cheng, Erik Deumens, Xiaguang Zhang, Ajith Perera, John F. Stanton

# QTP Faculty 1999





QTP Faculty 2006

# QTP is special

- The best innovators in electronic structure and dynamics and the mathematics applied to study molecular level processes in chemistry, physics, and biology are at QTP by choice
- Such as Frank Harris



# QTP since its start at the forefront of Computing



# RETIRED AND STILL ACTIVE FRIENDS LIVING HISTORY

- HENK
- JACK
- DAVID
- SAM
- YNGVE
- (POL, JCS, CHARLIE, MIKE)