Institut de Química Teòrica i Computacional

EXCELENCIA MARÍA DE MAEZTU

CICLE DE CONFERÈNCIES IQTCUB 2020

Paul S. Bagus (Univesity of North Texas)

22 de gener de 2020, Aula Enric Casassas 11:30 h

Paul Bagus és un dels pioners de la química quàntica. Va fer el doctorat al grup d'en Robert Mulliken (Premi Nobel de Química 1966) sota la supervisió de Clemens Roothaan. Bagus i Roothaan són els desenvolupadors del primer mètode Hartree-Fock per a capes obertes que mantenia la multiplicitat de espín.

Golden Years In The Development of Quantum Chemistry at Chicago (LMSS) and San Jose (IBM):

Lessons That are Relevant Today

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Presentations at the 1959 Boulder conference on Molecular Quantum Mechanics showed the potential of rigorous non-empirical, *ab initio*, quantum chemical calculations to address and solve chemical problems. About 25% of the papers in the conference proceedings, published in Reviews of Modern Physics, were contributions from the Laboratory of Molecular Structure and Spectra, LMSS, directed by Roothaan and Mulliken, at the University of Chicago. During the 1960's several people from LMSS moved to Clementi's department at the IBM Research Laboratory in San Jose, California to continue the development and application of programs for the calculation of Hartree-Fock and correlated wavefunctions. Because of limitations of available computers calculations often had to be individually designed to contain the correct chemistry and still be computationally feasible. An important focus of the early work was to establish conceptual understanding through computation rather than only to obtain a numerical result for some property. A selection of work from LMSS and IBM San Jose will be reviewed. It will be shown that the ideas and concepts that were established then are still relevant for the most profitable use of computational theory.