

Introduction to Gaussian: Theory and Practice

- Actualizado (16.09.2005)

SPAIN, in conjunction with CESCA.

Date: September 12-15, 2000

Location: CESCA- Centre de Supercomputació de Barcelona

Edifici Nexus

Gran Capita, 2-4

Barcelona, SPAIN

JAPAN, in conjunction with COMPAQ

Date: October 3-6, 2000

Location: Compaq JAPANHeadquarters

Tennonz Higashi Shinagwa,

Shinagawa-ku Tokyo JAPAN

"Introduction to Gaussian: Theory and Practice." will be presented by representatives of Gaussian, Inc.

The workshops will cover the full range of methods available in the Gaussian 98 package with emphasis on new methods and features which make Gaussian 98 applicable to an ever widening spectrum of research applications.

The workshop is structured to provide an introduction to electronic structure theory as well as a hands-on review for researchers active in the field. The workshop is open to researchers at all levels of academic, government and industrial research.

Preliminary Topic List:

Independent Particle Methods

Model Chemistries: A Framework for Understanding Electronic Structure Theory Results

Using ONIOM

MCSCF Methods and Applications

Geometry Optimization Techniques

Electron Correlation Methods

Density Functional Theory Methods

Methods for Excited Electronic States

Interpretation of Gaussian Results

Prediction of Molecular Properties

Solvent Effects via Electronic Structure Methods

Estimating Resource Requirements

There will be hands-on sessions each day between the morning and afternoon

lectures. Additional hands-on sessions will be available until the building closes. Workshop participants will be provided with use of a workstations to complete exercises, experiment and/or conduct short research topics.

The GaussView user interface will be used to perform visualization of results and to facilitate calculation setup. Each workshop participant will also be provided a copy of the lecture notes, a copy of Exploring Chemistry with Electronic Structure Methods, 2nd Edition, and a Gaussian 98 User's Reference.

For an Application please contact (Please specify which workshop):

Workshop Coordinator Gaussian, Inc.

Caregie Office Park, Bldg. 6

Pittsburgh, PA 15106

Additional information can be obtained from:

Telephone: 412 279 6700

Fax: 412 279 2118

email: info@gaussian.com

COST: \$350.00 per person. Attendees will be responsible for meals and lodging.

Hotel Accommodations: A list of hotel accommodations in the vicinity of the the workshop location will be made available to all registrants.

Hotel accommodations will be the responsibility of each participant.

Meals: Meals will be the responsibility of each participant.

DEADLINES: Receipt of Registration Materials along with the registration fee must be received by: September 1, 2000 for the SPAIN Workshop and September 15, 2000 for the JAPAN workshop.

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