ΠΑΝΕΠΙΣΤΗΜΙΟ ΑΘΗΝΩΝ

ΤΟΜΕΑΣ ΦΥΣΙΚΗΣ ΣΤΕΡΕΑΣ ΚΑΤΑΣΤΑΣΗΣ

ΠΑΝΕΠΙΣΤΗΜΙΟΥΠΟΛΗ, 157 84 ΑΘΗΝΑ

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ΠΟΛΥΤΕΧΝΕΙΟΥΠΟΛΗ, 157 80 ΑΘΗΝΑ

ΣΕΜΙΝΑΡΙΑ
ΦΥΣΙΚΗΣ ΣΥΜΠΥΚΝΩΜΕΝΗΣ ΥΛΗΣ

Τετάρτη 19-1-2011 12:00

Αίθουσα 027, Ισόγειο Κτιρίου Φυσικής, Πολυτεχνειούπολη Ζωγράφου

Approximating electronic correlations with Reduced Density Matrix Functional Theory (RDMFT)

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In RDMFT, the one-body reduced density matrix (1-RDM) is the fundamental density i.e. it plays the same role as the electronic density in Density-Functional Theory (DFT). The obvious advantage is that the kinetic energy is a simple explicit functional of the 1-RDM. Consequently, no kinetic energy contributions exist in the exchange and correlation term. In RDMFT approximate expressions of the total energy are written in terms of the 1-RDM and minimized with respect to 1-RDM under the N-representability conditions which guarantee that the optimal 1-RDM corresponds to a many-body wave function.

RDMFT is only relatively recently exploited for realistic calculations in molecules and solids. We review the basic ideas of RDMFT, the most important functionals and promising applications to prototype finite and periodic systems. These applications include calculations of dissociation energy plots, atomization energies, ionization potentials, the fundamental gap of semiconductors and insulators, as well as the calculation of the correlation energy of the homogeneous electron gas.

The aim of developing RDMFT is not to replace a well established and widely used theory, like DFT, but to develop an efficient method that could give answers to problems for which DFT results deviate from experiment.

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