ΙΔΡΥΜΑ ΤΕΧΝΟΛΟΓΙΑΣ ΚΑΙ ΕΡΕΥΝΑΣ

ΣΕΜΙΝΑΡΙΟ

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ΘΕΜΑ: **HYPERPOLARIZABILITIES OF PUSH-PULL POLYENES**

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΕΙΧΗΜΥΘ-ΙΤΕ

ΗΜΕΡΟΜΗΝΙΑ: Τρίτη, 9 Σεπτεμβρίου 2003

ΩΡΑ: 19:00

ΠΕΡΙΛΗΨΗ

Static as well as dynamic electronic and vibrational longitudinal first hyperpolarizabilities of α, ω -nitro,amino-polyacetylene oligomers have been computed at the Hartree-Fock and second-order Møller-Plesset levels using the 6-31G atomic basis set. The curve of first hyperpolarizability per unit cell versus the number of unit cells defines the optimal chain length for NLO applications. Modifications in electronic structure occurring when electron correlation is included lead to an increase in the height of the maximum by a factor of two. A similar enhancement arises from the corresponding change in equilibrium geometry which, in addition, shifts the position of the maximum towards longer chain lengths. Frequency dispersion also has a major effect on the position and magnitude of the optimal point while contributions from the vibrational hyperpolarizability is relatively small when correlation and frequency dispersion are included.