**Molecular modeling studies of mass transport process in azobenzene materials**

L.E. Epure1, S. Ciobotarescu1, V. Teboul2, N. Hurduc1

1. "Gheorghe Asachi" Technical University of Iasi, Department of Natural and Synthetic Polymers, Prof. Dimitrie Mangeron Street, 73, 700050-Iasi, Romania
2. Faculty of Sciences, University of Angers, 2 Bd. de Lavoisier, 49000 Angers, France

Azo-polymers are part of the “intelligent materials family” because they are able to change the configuration, elasticity, or other mechanical parameters using only the light as an external stimulus.

Using of a polarized laser source can generate surface relief gratings on the film surface used as cell culture support. Azobenzenes undergo an isomerization process, passing from the stable trans configuration, toward the less stable geometric isomer, cis. Large conformational changes are associated with the trans-cis photochemical isomerization of azobenzenes.

Understanding and manipulating these reordering phenomena at the molecular level is beneficial for the applications of azopolymers in the bio-field. Valuable information can be obtained through molecular modeling studies. Using this method we are trying to understand the mechanism that originates from the mass transport process which takes place in azobenzene materials.

# Biography

Luiza Epure has completed his Ph.D. in 2012 at Gheorghe Asachi Technical University of Iasi. She works at the Department of Natural and Synthetic Polymers from Faculty of Chemical Engineering and Environmental Protection. She does research in polymer and computational chemistry.

lepure@tuiasi.ro