

# INTERMOLECULAR INTERACTIONS IN AZOCOMPOUNDS: A FIRST-PRINCIPLES DENSITY FUNCTIONAL APPROACH

Abulyaissova L.K., Boribayeva A.M., Aitan M.

*Academician Ye.A. Buketov Karaganda State University,  
Karaganda, Kazakhstan  
lyazzat.kz07@mail.ru*

The well-known classes of azocompounds such as Schiff-bases and azobenzenes are used as mesogenic substances. Mesogenic (liquid crystalline) properties are associated with the processes of molecular aggregation.

In this work, we report a theoretical study on molecular structure of the entitled thermotropic liquid crystals using the density functional theory (DFT) approach. We have simulated and studied the molecules with electron-donating, electron-withdrawing substituents in the para-position of aryl rings and reference unsubstituted azocompounds. Possible options for the relative position of a pair of molecules for stacking, plane and terminal interactions were considered. We aim to analyze the relative stabilities of several different dimeric associates, and to report theoretical results regarding an intermolecular interaction energy, HOMO-LUMO energies and their energy gaps, etc.

Interaction energy of molecules in the dimers of various configurations and other physico-chemical properties are calculated at the affordable B3LYP/3-21G, B3LYP/6-31G (with polarization and diffuse functions) levels of theory.

The structure of azocompound molecules in the isolated state is optimized by quantum chemical calculations with the 6-31G(d,p), 6-31++G(d,p) basis sets. The geometry of dimers have been calculated at the B3LYP/3-21G level.

The results show that for short-range order the energy and thermodynamic stabilities of the dimers depend on the intermolecular distance, relative orientation, structure and physical characteristics (dipole moment, polarizability, etc.).