

POTENTIAL ENERGY SURFACE ANALYSIS OF PHOTOCROMIC COMPOUND BASED ON QUANTUM-CHEMICAL COMPUTATION

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Many physical properties of photoactive molecular systems are related in one way or another to the electronic energy spectrum of the system. Vertical excitation energy from the ground state to some excited state is commonly assumed to match – or used to estimate – the wavelength of the absorption peak. Similarly, vertical excitation energy to certain excited state is expected to correspond to the luminescence wavelength if the geometric structure of a system is optimized for that particular state. Such optimization itself is usually performed as a gradient minimum search in multidimensional space – *potential energy surface* (PES) of a molecular system.

With some knowledge of the PES, additional properties can be estimated. Those properties include the type of structural deformations during the photo-excitation process and even some dynamical parameters (the simplest being reaction rate between two molecular conformations separated by an energy barrier). Thus, knowing the shape of the PES for various electronic states is extremely useful. However, obtaining sufficient information, especially for excited states, is a difficult and computationally intensive task. Practical approaches to the problem often require certain restrictions, partial knowledge of the system at hand, and human insight in general.

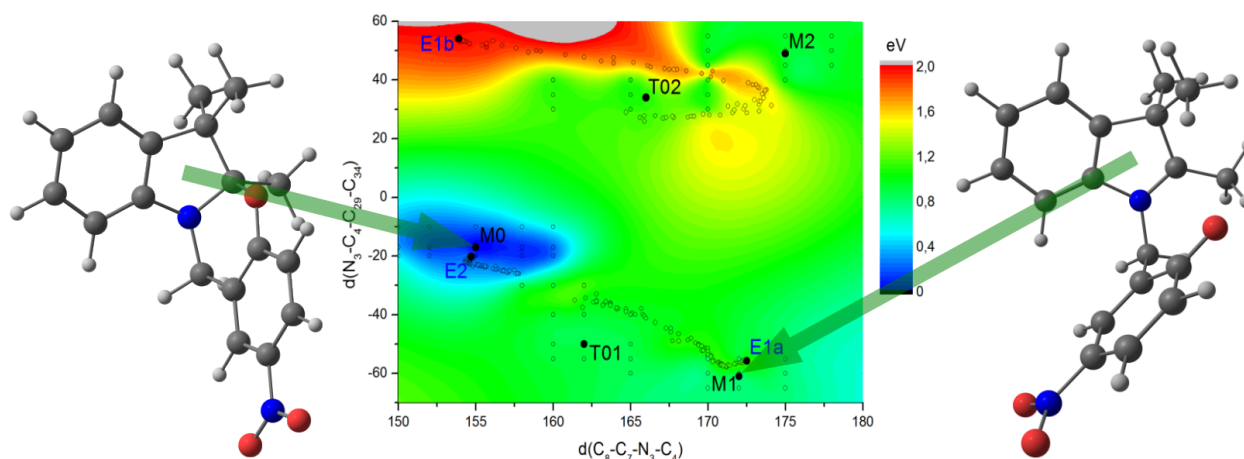


Fig. 1. The ground-state potential energy surface of the IB compound as a function of two dihedral angles [1].

This presentation is based on quantum-chemical study of photochromic indolo-benzoxazine compound (Fig. 1, left and right) [1]. Results of various computations and ways to use them to identify the structure of the PES (ground-state surface is shown in Fig. 1, middle) will be discussed.

[1] S. Toliautas, J. Sulskus, L. Valkunas, M. Vengris, Quantum chemical studies of photochromic properties of benzoxazine compound, *Chemical Physics* **404**, 64-73 (2012).