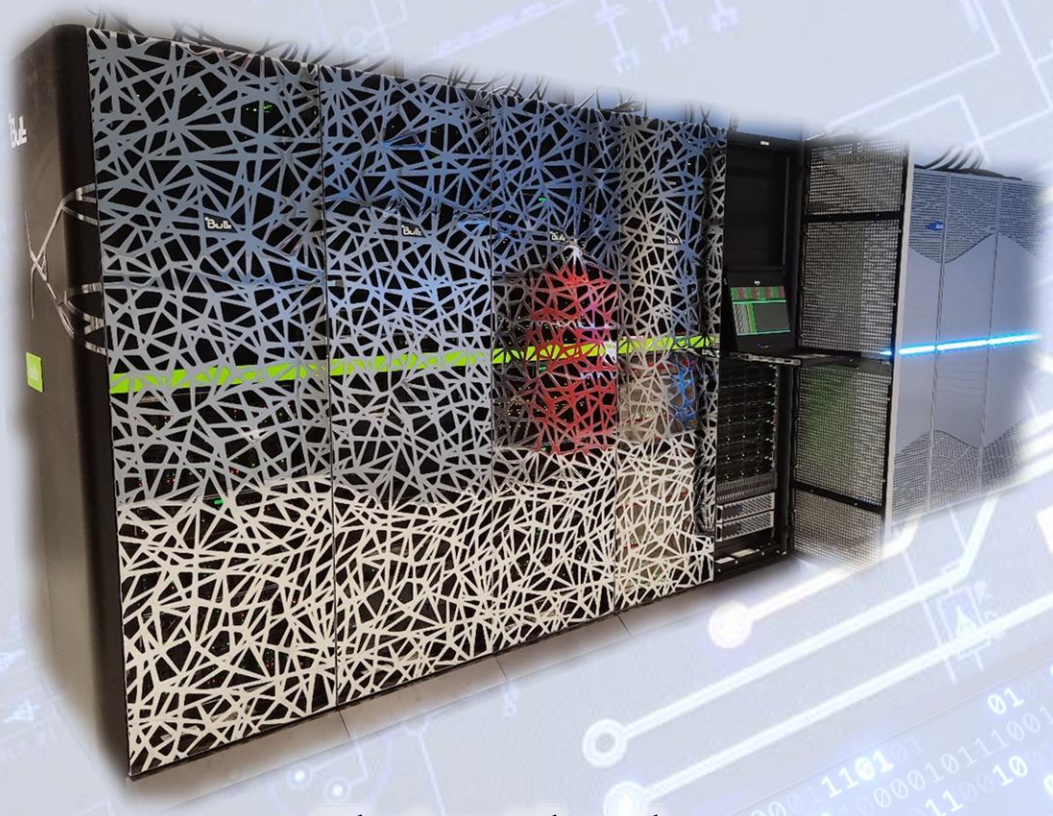
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

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Vilniaus universitetas 1579 Universitas Vilnensis — Matematikos ir informatikos fakultetas

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Derivatives of Enamines as *p*-type Semiconductors. Structure and Energetics using QC approach

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Organic hole-transporting materials (HTMs) are important as a photo-voltaic sensor for different purposes: *in vivo* sensors for biological systems [1], perovskite solar cells [2], etc. This work represents the investigation of structure and energetical properties of the hole transporting enamine units (central core) related to the spiro-bis-indane-based compounds by combining different aniline substituents [3], see Fig.1. Ground state energy structure and following electronic excitations were obtained using *Gaussian16* [4] package. Density functional theory (DFT) Cam-B3LYP method and 6-31G(d) basis set (supplemented with polarization functions (d)) were used for ground-state optimization that supplemented the experimental study. Due to the large volume of molecular structures, solvation effects were not considered in all cases. Semiempirical TD method (for singlets only) was used for estimation of parameters of Frank-Condon type transition and corresponding charge redistribution. Several molecular realizations of promised conformers are presented in Fig. 2. Substituents are oriented in a chaotic manner resulting in a vast array of different conformers. All structures were derived using the *grad-optimization* technique, ensuring convergence of all parameters such as Maximum Force, RMS Force, Maximum Displacement and RMS Displacement. Both HTMs exhibited high thermal stability and relatively high hole-drift mobility, making them viable candidates for application as HTMs.

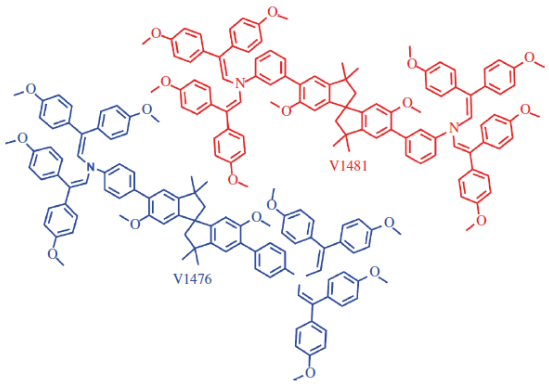

Fig. 1. Structures of HTMs V1476 and V1481.

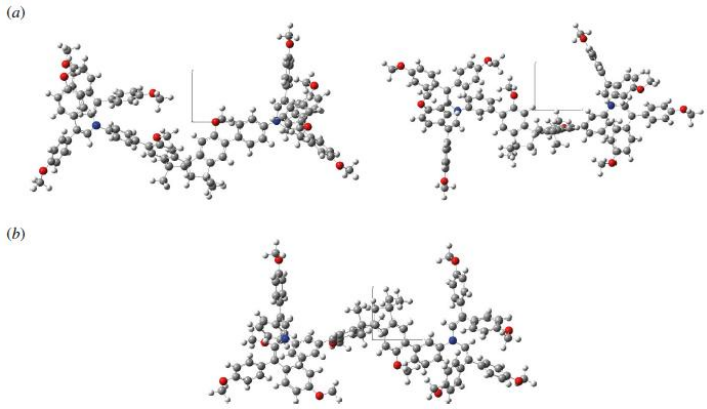

Fig. 2. Most promised conformers of V1476 (a) and V1481 (b).

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