Abstract:
This work is focused on the properties of polyaniline placed on the model of silicate surface, namely its adhesion energy and spectra of polyaniline with different charge, computed by means of quantum chemistry. Computed spectra were compared with experimental data. The DFT metod ω-B97XD with 3-21G base was used for optimalization of the complex model and for determination of vibrational spectra the DFT metod ω-B97XD with 6-31G(d,p) base was used. Evaluation of the adhesion energy DFT metod ω-B97XD with 6-31G* base was used. The adhesion energy computed by interpolation to infinite polymer was 1,9kcal/mol. Computed Raman spectra was fit to experimental data. Spectrum found by this metod was similar to experimental in some aproximation, but more detail look would reavel some differences caused by not including of enviroment and of interaction between polyaniline