

## Abstract

The doctoral dissertation concerns the possibility of functionalization of molecules and the study of changes in their physicochemical properties by computational chemistry methods. It has been evaluated that the combination of the magnetic properties of transition metal oxides (FeO, NiO, CoO) with the reducing capacity of alkali metals (Li, Na and Li<sub>2</sub>, Na<sub>2</sub>) are leading to form modified oxides which are characterized by very low ionization potential values (in the range of 4,85–3,96 eV) whereas their magnetic properties are being preserved (the local spin magnetic moments at the transition metals span 0,8–4,9  $\mu_B$  range). It has been revealed that the modification of alkaline earth metal oxides (BeO, MgO and CaO) by alkali metal oxides (Li<sub>2</sub>O, Na<sub>2</sub>O and K<sub>2</sub>O) results in the formation of stable mixed oxides whose acid-base properties were estimated by calculation of proton affinity (PA), gas-phase basicity (GPB) and hydride affinity (HA), and gas-phase electrophilicity (GPE). In particular, the basicity of such designed systems increases with an increase in the atomic number of alkali metals (in the series of MOLI<sub>2</sub>O < MONa<sub>2</sub>O < MOK<sub>2</sub>O (where M=Be, Mg, Ca)). Furthermore, it was presented that the Lewis acidity of the corresponding [MON<sub>2</sub>O]H<sup>+</sup> determined with respect to hydride anion decreases as the basicity of the corresponding oxide increases. It has been also described that the functionalization of the BH<sub>3</sub>, AlH<sub>3</sub> and GaH<sub>3</sub> by the elements of the alkaline earth metals (M' = Mg, Ca) leads to formation of stable molecules bonded by dative bond arising from donation of an  $ns^2$  electron pair on an alkaline earth atom (Mg or Ca) into a vacant  $n'p$  orbital on the group 13 atom of hydrides. In addition, it has been analysed what happens when an excess electron is attached to form corresponding molecular anions.