

Anawat Thivasasith 2010: DFT Study of the Gas-Selective Metallopolymers.  
Master of Science (Chemistry), Major Field: Chemistry, Department of  
Chemistry. Thesis Advisor: Mr. Pipat Khongpracha, Ph.D. 70 pages.

Density functional theory using the B3LYP functionals was performed to investigate NO, CO, NO<sub>2</sub> and O<sub>2</sub> gas-selective property of the metal-containing conductive polymer. The complexes of Co, Ni and Cu with N,N'-propylenebis (salicylideneimine) ligand (salpn) and modification 3,4-(ethylenedioxy)thiophene ((salpn)-EDOT) were modeled as their active center for molecular gas sensing. All the metal active centers were assigned to have low spin state. The optimized geometry of the Co(II)(salpn) complex is considered to be distorted square planar while that of Ni(II)(salpn) and Cu(II)(salpn) complexes are square planar. The adsorption of NO, CO, NO<sub>2</sub> and O<sub>2</sub> onto the metal active center disturbed their local geometry. Co, Ni and Cu active centers adopt distort square pyramidal geometry in the adsorption complex. The adsorption energy for Co(II), Ni(II) and Cu(II)(salpn)/NO are about -10.47, -10.43 and -4.28 kcal/mol, respectively. When modification EDOT in to metal(II)(salpn) is slightly enhances their adsorption energy. The adsorption energy for Co(II), Ni(II) and Cu(II)(salpn)-EDOT are about -13.33, -10.56 and -5.39 kcal/mol, respectively. The results, were vary gas such as CO, NO<sub>2</sub> and O<sub>2</sub> onto the metal(II)(salpn)-EDOT. The adsorption energy for Co(II)(salpn)-EDOT/CO, NO<sub>2</sub> and O<sub>2</sub> are about -4.88, -14.13 and -3.98 kcal/mol, respectively. The adsorption energy for Ni(II)(salpn)-EDOT/CO, NO<sub>2</sub> and O<sub>2</sub> are about -5.82, -19.76 and -4.57 and Cu(II)(salpn)-EDOT/CO, NO<sub>2</sub> and O<sub>2</sub> are about -3.67, -20.17 and -4.01. The adsorption of gas molecule onto metal active center significantly reduces the energy gap of the complex for NO and NO<sub>2</sub> molecules, and thus enhances their electrical conductivity.

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