ABSTRACT

ADSORPTION of PLATINUM OXIDE (PtO) and PLATINUM DIOXIDE (PtO2) CLUSTERS on MONOLAYER ALUMINIUM NITRIDE

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In this thesis, we first investigate the adsorption properties of single Pt and O atoms and PtO, PtO_2, and Pt_2O clusters on hexagonal AlN monolayer. We employ density functional theory (DFT) to study electronic structure and charge transfer of h-AlN by considering nonmagnetic (NM) and ferromagnetic (FM) states. PtO and Pt_2O adsorbed h-AlN system has FM ground state with 2.00 m_B magnetic moment, while PtO_2, Pt, and O adsorption lead to NM structures. Pt adsorbed AlN system has the lowest adsorption energy with -3.175 eV indicating the most stable structure energetically.

These properties can lead to possible applications in spintronics and nano electronic devices.

Key words: Density functional theory (DFT), monolayer AlN, small Platanium clusters