

## ABSTRACT

### ADSORPTION of PLATINUM OXIDE (PtO) and PLATINUM DIOXIDE (PtO<sub>2</sub>) CLUSTERS on MONOLAYER ALUMINIUM NITRIDE

Aynur AKÇAY

M.Sc. Thesis, Department of Physics  
Supervisor: Assoc. Prof. Dr. Ethem AKTÜRK  
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In this thesis, we first investigate the adsorption properties of single Pt and O atoms and PtO, PtO<sub>2</sub>, and Pt<sub>2</sub>O 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<sub>2</sub>O adsorbed h-AlN system has FM ground state with 2.00 m<sub>B</sub> magnetic moment, while PtO<sub>2</sub>, 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 Platinum clusters