DOI: doi.org/10.47363/JPSOS/ICWOQ2025/2025(7)7

International Conference on
Wave Equations, Optical Engineering and Quantum Mechanics (ICWOQ-2025)

Conference Proceedings April 25, 2025 - Barcelona, Spain

Dissociation of O_2 Molecule ON MO_4, MO_3(PT, PD, RE AND NI) Clusters for PEM Fuel Cell - Study DFT

Karen De la Mora

Department of Theoretical, Atomic and Optical Physics, Spain

The present study focused on the adsorption and dissociation of O_2 on Mo_4 clusters and Mo_3(M) is investigated the doping of (Pt, Pd, Re and Ni) atoms in Mo_3 clusters. The dissociation of the molecule O_2 on metal clusters are of fundamental interest for several reaction catalytic in the cathode of a PEM Fuel Cell. The calculations are carried out on Density-Functional Theory DFT for the adsorption and dissociation of O_2 on Mo_4, Mo_3(Pt, Pd, Re and Ni) clusters. Molecular electrostatic potential (MESP), partial density of states (PDOS), and characteristics was employed the transition states (TS) to search The Reaction Kinetics of the species. In addition, vibration frequency calculations were performed to verify whether each species is a minimum or a transition state on the potential energy surfaces; this is were employed for understanding the interaction characteristics. The calculations are carried out on Density-Functional Theory DFT - Dmol3- Material´s Studio.