**Abstract**

**Chemistry (CH)**

**Title: Electrocatalytic CO2 reduction reaction for carbon dioxide conversion to high valued added compounds on transition metal embedded graphene-based material: A theoretical study**

**CH####**

**Field:** Chemistry

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**Abstract:**

Nowadays, the world is facing the challenge of greenhouse gasses and climate change, so it is more important than ever to develop solutions that reduce carbon dioxide (CO2). The electrochemical CO2 reduction reaction (CO2RR) is one of the most popular methods for the conversion of CO2 into high-value products. Graphene surfaces are an interesting catalyst for the CO2RR reaction due to their unique electrochemical and structural characteristics. In this work, we investigated the adsorption of CO2 molecules on transition metals (TM =Cu, Pt, and Pd) decorated graphene surfaces (Cu-, Pt-, and Pd-B2N4-graphene) using density functional theory (DFT) calculations. Our findings reveal that these TM-decorated graphene surfaces (Cu-, Pt-, and Pd-B2N4-graphene) demonstrate strong binding energies (Eb) of -7.02, -9.53, and -7.49 eV, respectively and From the absorption energy (Eabs) of CO2 on surfaces, it can be seen that the energy used to adsorb CO2 onto surfaces is most effective in Pt-B2N4-graphene (-9.53 eV) > Pd- B2N4-graphene (-7.49 eV) > Cu- B2N4-graphene (-7.02 eV). These results indicate a consistent trend across both sets of data. In the future, we will absorb various molecules according to the mechanism of CO2RR to observe and calculate the efficiency of CO2RR reactions on our surfaces. Therefore, we hope that TM-B2N4-graphene might be a high-performance catalytic material for highly effective material for CO2RR reaction.

**Keywords:** Electrochemical CO2 Reduction, transition metals (TM), Density functional theory (DFT), binding energies