# Computational screening of trimetallic alloy cluster decorated on N-Gr for $CO_2$ activation and conversion

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The electrochemical reduction of $CO_2$ offers a promising pathway for the sustainable production of carbon-neutral fuels and value-added chemicals; however, the rational design of highly efficient and selective catalysts remains a significant challenge. In this work, we present a comprehensive first-principles screening of trimetallic alloy clusters supported on nitrogen-doped graphene (N–Gr) for $CO_2$ reduction, employing density functional theory (DFT) to elucidate the underlying structure–activity relationships. The synergistic interaction among the constituent elements in the alloy modulates the physicochemical properties of the catalyst and governs its catalytic performance [1]. We systematically investigated MoTi-based triatomic alloy clusters in which the third element was selected from a diverse set of transition metals (Fe, Co, Cu, Ru, Rh, Pd, Pt, Ag, Au, and Ir). Among the studied systems, all models except those containing Cu, Ru, Rh, and Ir exhibited strong $CO_2$ activation. Using the computational hydrogen electrode (CHE) model [2], the reaction energetics toward C1 products were evaluated and the most favorable reaction pathways were identified. This study provides fundamental insights into the synergistic effects among the metal atoms and offers a rational strategy for the design of high-performance electrocatalysts for $CO_2$ reduction.

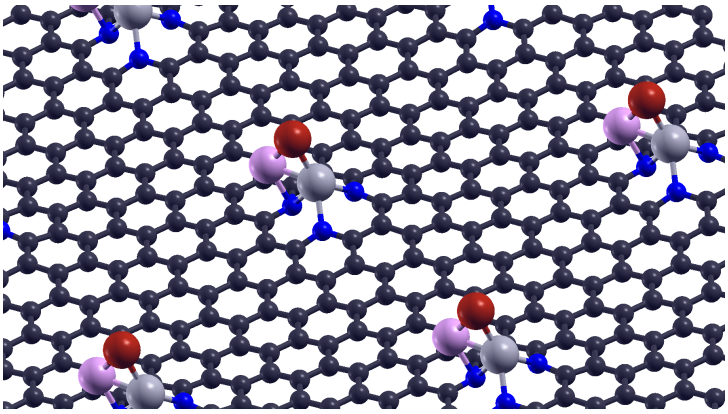

**Figure 1:** Geometrical representation of MoTiTM trimetallic clusters supported on N3-doped graphene (TM = Fe, Co, Cu, Ru, Rh, Pd, Pt, Ag, Au, and Ir), highlighting the atomic arrangement and metal–nitrogen coordination at the catalytic active site.

## References

[1] Ning, Shuying, Nini Wen, Bingtao Zhao, Muhammad Kashif, Philippe M. Heynderickx, and Yaxin Su. *ACS Applied Materials & Interfaces* 16, no. 47 (2024): 64664- 64680.
[2] Peterson, Andrew A., Frank Abild-Pedersen, Felix Studt, Jan Rossmeisl, and Jens K. Nørskov. *Energy & Environmental Science* 3, no. 9 (2010): 1311-1315.