

N₂O+CO reaction over single Ga or Ge atom embedded graphene: A DFT study

Mehdi D. Esrafil, Esmail Vessally

PII: S0039-6028(17)30409-0
DOI: [10.1016/j.susc.2017.10.001](https://doi.org/10.1016/j.susc.2017.10.001)
Reference: SUSC 21103



To appear in: *Surface Science*

Received date: 3 June 2017
Revised date: 9 August 2017
Accepted date: 2 October 2017

Please cite this article as: Mehdi D. Esrafil, Esmail Vessally, N₂O+CO reaction over single Ga or Ge atom embedded graphene: A DFT study, *Surface Science* (2017), doi: [10.1016/j.susc.2017.10.001](https://doi.org/10.1016/j.susc.2017.10.001)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Highlights

- The $\text{N}_2\text{O} + \text{CO}$ reaction is studied on the single Ga or Ge atom embedded graphene.
- The catalytic activity of the Ge-embedded graphene for $\text{N}_2\text{O} + \text{CO}$ reaction is larger than that of Ga-embedded one.
- The disproportionation of N_2O molecule does not occur on these surfaces at normal temperature.

ACCEPTED MANUSCRIPT

Download English Version:

<https://daneshyari.com/en/article/5421074>

Download Persian Version:

<https://daneshyari.com/article/5421074>

[Daneshyari.com](https://daneshyari.com)