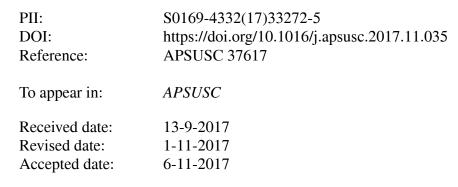
### Accepted Manuscript

Title: First row transition metal atoms embedded in multivacancies in a rippled graphene system

Authors: Dominique Mombrú, Ricardo Faccio, Alvaro W. Mombrú



Please cite this article as: Mombrú D, Faccio R, Mombrú AW, First row transition metal atoms embedded in multivacancies in a rippled graphene system, *Applied Surface Science* (2010), https://doi.org/10.1016/j.apsusc.2017.11.035

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.



### ACCEPTED MANUSCRIPT

# First row transition metal atoms embedded in multivacancies in a rippled graphene system

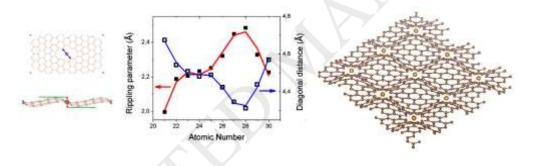
Dominique Mombrú<sup>1</sup>, Ricardo Faccio<sup>1</sup>, Alvaro W. Mombrú<sup>1,\*</sup>

<sup>1</sup>Centro NanoMat, Cryssmat-Lab, DETEMA, Facultad de Química, Universidad de la República, Montevideo, Uruguay

\*Author to whom all correspondence should be addressed

E-mail: amombru@fq.edu.uy

Graphical abstract



#### Highlights

- . DFT study of a transition metal atom embedded in an 8-order multivacant graphene.
- . Rippling of such systems is the same as the one observed for the metal-less system.
- A correlation between the distortion in the *ab* plane and the rippling has been found.
- . Systems with metal atoms have lower magnetic moments than the metal-less system.
- . Quenching of the magnetic moment is observed for Sc and Cu.

Download English Version:

## https://daneshyari.com/en/article/7835824

Download Persian Version:

https://daneshyari.com/article/7835824

Daneshyari.com