

Article

# Electronic Supplementary Information for the article “Tuning the Magnetic Moment of Small Late 3d-Transition-Metal Oxide Clusters by Selective Mixing the Transition-Metal Constituents.”

Rodrigo H. Aguilera-del-Toro<sup>1</sup>  , María B. Torres<sup>2,\*</sup>  , Faustino Aguilera-Granja<sup>3</sup>  and Andrés Vega<sup>1</sup> 

<sup>1</sup> Departamento de Física Teórica, Atómica y Óptica, Universidad de Valladolid, Valladolid 47011, Spain; rodrigohumberto.aguilera@uva.es (R.H.A.-d.T.); avega@fta.uva.es (A.V.)

<sup>2</sup> Departamento de Matemáticas y Computación, Universidad de Burgos, Burgos 09006, Spain; begonia@ubu.es (M.B.T.)

<sup>3</sup> Instituto de Física, Universidad Autónoma de San Luis Potosí, San Luis Potosí 78290, México; faustino@ifisica.uaslp.mx (F.A.-G.)

\* Correspondence: begonia@ubu.es

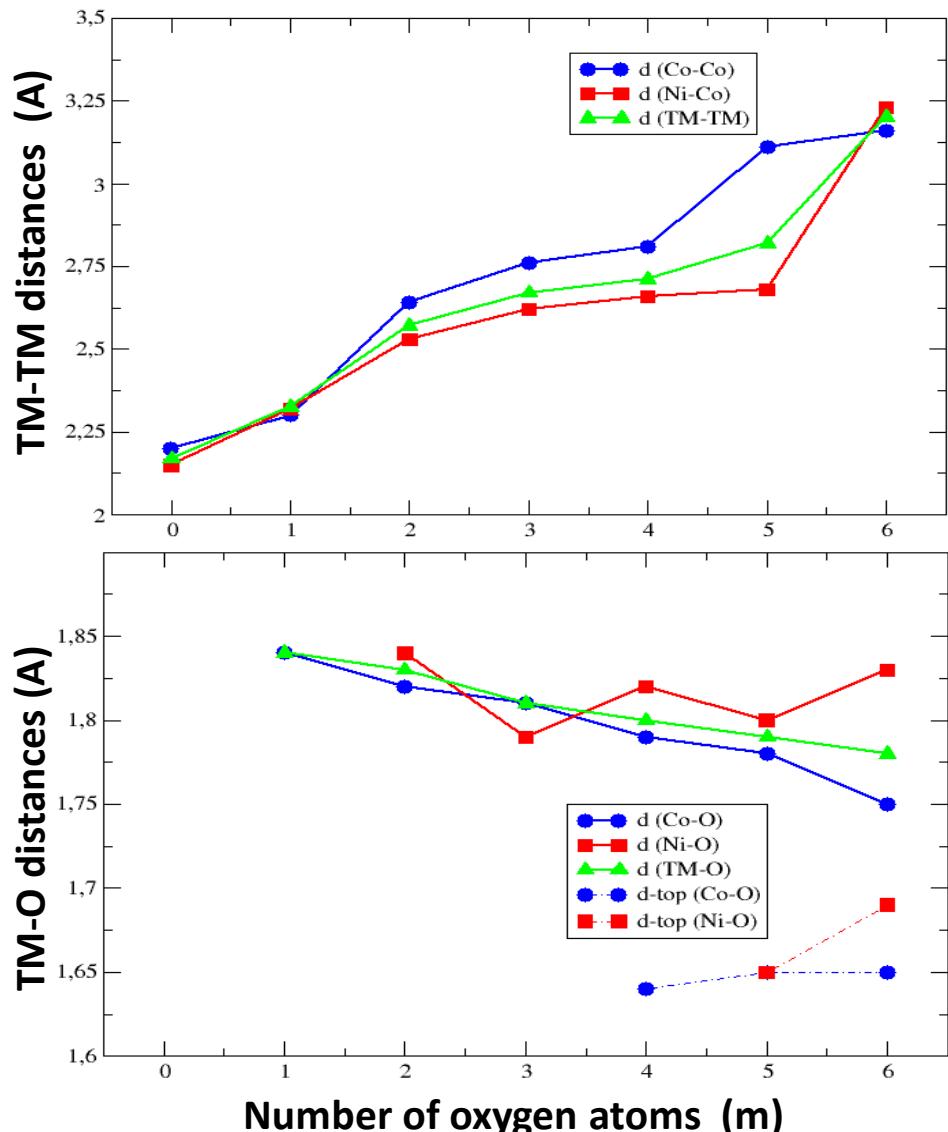
Version September 10, 2020 submitted to Nanomaterials

**Keywords:** magnetism; transition-metal oxide clusters; DFT calculations; structure; electronic properties;

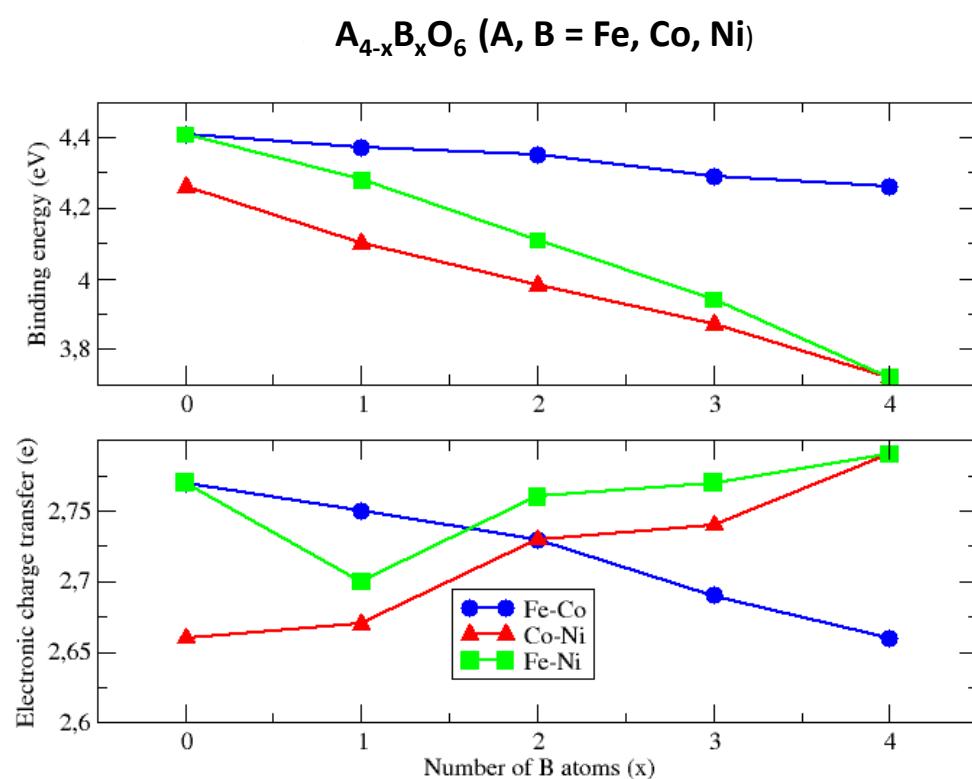
**PACS:** 75.75+a; 36.40Cg; 75.30.Pd; 75.50.-y

---

© 2020 by the authors. Submitted to *Nanomaterials* for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).



**Figure 1.** (Color online) **(a)** Upper panel: average TM-TM distance (green), Co-Co distance (blue), and average Co-Ni distance (red) for  $\text{Co}_2\text{Ni}_1\text{O}_m$  oxides as a function of the number of oxygen atoms,  $m$ . **(b)** Lower panel: average TM-O distance (green), average Co-O distance (blue), and average Ni-O distance (red) for  $\text{Co}_2\text{Ni}_1\text{O}_m$  oxides as a function of the number of oxygen atoms,  $m$ . Continuous (dashed) lines correspond to average distances between oxygens on bridge (top) positions and TM atoms.



**Figure 2.** (Color online) Binding energies in eV (upper panel) and average electronic charge transfer in  $e$  (lower panel) of  $A_{4-x}B_xO_6$  ( $A, B = Fe, Co, Ni; x = 0 - 4$ ) oxides. Blue, green and red curves correspond to Fe-Co, Fe-Ni and Co-Ni nanoalloys, respectively.