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**Garcia-Fernandez, P.; Aramburu, J.A.; García Lastra, Juan Maria; Moreno, M.**

*Publication date:*  
2016

*Document Version*  
Early version, also known as pre-print

[Link back to DTU Orbit](#)

*Citation (APA):*

Garcia-Fernandez, P., Aramburu, J. A., García Lastra, J. M., & Moreno, M. (2016). Evidence of a Jahn-Teller impurity in a cubic lattice displaying a compressed geometry. Abstract from International Conference on Defects in Insulating Materials 2016, Lyon, France.

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## ABSTRACT SUBMISSION FORM

# Evidence of a Jahn-Teller impurity in a cubic lattice displaying a compressed geometry

P. García-Fernández<sup>1</sup>, J. A. Aramburu<sup>1</sup>, J. M. García-Lastra<sup>2</sup>, and Miguel Moreno<sup>1</sup>

<sup>1</sup> *Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Universidad de Cantabria, Avenida de los Castros s/n, 39005 Santander, Spain*

<sup>2</sup> *Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark*

Spontaneous symmetry-breaking around a defect site leads to interesting quantum phenomena, like tunnelling between various stable wells that, under the correct conditions could serve as the basis for applications like quantum computation<sup>1,2</sup>. Of particular interest is the Jahn-Teller distortion appearing in some transition-metal impurities in cubic lattices that usually involves the elongation of the metal ligand octahedron along one of its axes. For a long time it was believed that this was the case for a nickel-associated defect appearing in CaO:Ni<sup>2+</sup> after irradiation<sup>3</sup>, ascribed to a Ni<sup>3+</sup> (3d<sup>7</sup>) ion with a S=1/2 ground state<sup>4</sup>. First principle calculations together with an analysis of experimental data found for 3d<sup>9</sup> and 3d<sup>7</sup> ions in cubic oxides prove however that the centre found in irradiated CaO:Ni<sup>2+</sup> corresponds to Ni<sup>+</sup> under a static Jahn-Teller effect displaying a compressed equilibrium geometry<sup>5</sup>. To our knowledge this is the first genuine Jahn-Teller system (i.e. where exact degeneracy exists at the high-symmetry configuration) exhibiting compressed equilibrium geometry. Moreover, the present calculations<sup>5</sup> demonstrate that the anomalous positive g<sub>||</sub>-shift (g<sub>||</sub> - g<sub>0</sub> = 0.065) measured<sup>3</sup> at T = 20 K obeys to the superposition of |3z<sup>2</sup>-r<sup>2</sup>⟩ and |x<sup>2</sup>-y<sup>2</sup>⟩ states driven by quantum effects associated with the zero-point motion, a mechanism firstly put forward by O'Brien<sup>6</sup> and that, so far, had no rigorous experimental support. In the present case, that mechanism is shown to be enhanced by the low Jahn-Teller barrier (8.7meV) among equivalent configurations<sup>5</sup>. Finally an analysis of calculated energy barriers for different Jahn-Teller systems<sup>2,5</sup> allows us to explain the singular origin of the compressed geometry present in CaO:Ni<sup>+</sup>.

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