

Abstract Submitted  
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**Dynamical Jahn-Teller Effect and Antiferromagnetism in insulating Cs<sub>3</sub>C<sub>60</sub>** NAOYA IWAHARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven, Celestijnenlaan 200F, B-3001, Leuven, Belgium — The dynamical Jahn–Teller effect on fullerene sites in insulating Cs<sub>3</sub>C<sub>60</sub> is investigated fully *ab initio* [1]. The vibronic excitations of rotational type are at  $\geq 65$  cm<sup>-1</sup>, while the net kinetic contribution to the Jahn–Teller stabilization energy constitutes ca 90 meV. This means that no localization of distortions by intermolecular interactions is possible in these fullerenes, therefore, free rotations of deformations take place independently on each C<sub>60</sub>. The latter destroy the orbital ordering and establish a conventional exchange interaction between  $S = 1/2$  on fullerene sites. The corresponding exchange model is derived and predicts the Néel temperature for A15 Cs<sub>3</sub>C<sub>60</sub> close to experiment.

[1] N. Iwahara and L. F. Chibotaru, Phys. Rev. Lett. **111**, 056401 (2013)

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