Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Dynamical Jahn-Teller instability in metallic fullerides NAOYA IWAHARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium — The ground state of metallic fulleride K_3C_{60} is investigated *ab initio* with a concomitant self-consistent treatment of the electron correlation and the Jahn-Teller (JT) effect [1]. The potential energy surface has two minima with and without JT distortion. It is found that static JT instability on C_{60} sites is favored when the intrafullerene electron repulsion $U > 650$ meV. At the same time the amplitude of variations of the band energy as function of the direction of JT distortions are found to be much smaller than the energy gain from dynamical delocalization of JT deformations implying dynamical JT instability on C_{60} sites. The latter develops already at $U = 500$ meV, while for $U > 600$ meV the amplitude of JT deformation approches the value for isolated C_{60}^{3-}, leading to strong enlargement and complete removal of degeneracy of the LUMO band.

[1] N. Iwahara and L. F. Chibotaru, submitted.

Naoya Iwahara
Theory of Nanomaterials Group, Katholieke Universiteit Leuven,
Celestijnenlaan 200F, B-3001 Leuven, Belgium

Date submitted: 15 Nov 2013 Electronic form version 1.4