

Abstract Submitted  
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**Dynamical Jahn-Teller effect in Cs<sub>3</sub>C<sub>60</sub> superconductors** LIVIU CHIBOTARU, NAOYA IWAHARA, None — The Cs<sub>3</sub>C<sub>60</sub> shows a superconducting critical temperature of 38K which is one of the highest among phonon-mediated superconductors. Recent infrared spectroscopy data of insulating Cs<sub>3</sub>C<sub>60</sub> apparently support the presence of Jahn-Teller dynamics in this fulleride [1]. To check this possibility, we have performed the DFT calculations of vibronic constants and multiplet splitting parameters, and have calculated from the first principles the spectrum of low-lying vibronic states on C<sub>60</sub><sup>3-</sup> sites by diagonalizing the full vibronic Hamiltonian in a large vibrational basis. The splitting of the t<sub>1u</sub><sup>3</sup> shell into degenerate multiplets and their vibronic mixing has been fully taken into account, as well as the effect of the environment on the local vibrations. The results show that in the insulating phase an unhindered dynamical Jahn-Teller effect takes place at each C<sub>60</sub> site. Using Gutzwiller approach in combination with LDA band structure, we demonstrate that the Jahn-Teller instability also persists in the metallic phase for a wide range of values of intrasite repulsion energy ( $U$ ).

[1] G. Klupp, P. Matus, K. Kamaras, A.Y. Ganin, A. McLennan, M.J. Rosseinsky, Y. Takabayashi, M.T. McDonald, K. Prassides, *Nat. Comm.* **2012**, *3*, 912.

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