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Orbital disproportionation of electronic density is a universal feature of alkali-doped fullerides NAOYA IWAHARA, LIVIU CHIBOTARU, Katholieke Universiteit Leuven — Alkali-doped fullerides A_nC_{60} show a remarkably wide range of electronic phases in function of A = Li, Na, K, Rb, Cs and the degree of doping, n = 1-5. While the presence of strong electron correlations is well established, recent investigations give also evidence for dynamical Jahn-Teller instability in the insulating and the metallic phase of A_3C_{60} [1, 2]. To reveal the interplay of these interactions in fullerides with even n, we address the electronic phase of A_4C_{60} with accurate many-body calculations within a realistic electronic model including all basic interactions extracted from first principles [3]. We find that the Jahn-Teller instability is always realized in these materials too. More remarkably, in sharp contrast to strongly correlated A_3C_{60}, A_4C_{60} displays uncorrelated band-insulating state despite pretty similar interactions present in both fullerides. Our results show that the Jahn-Teller instability and the accompanying orbital disproportionation of electronic density in the degenerate LUMO band is a universal feature of fullerides.
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