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First-principles calculation of electronic structures of new C_{60} polymers TAICHI KOSUGI, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo — C_{60} fullerene molecules form fcc crystalline structure at an ambient pressure and temperature. It has been both theoretically and experimentally confirmed that this structure undergoes phase transitions into various structures at high temperatures and high pressures. Yamanaka et al. experimentally found that the individual C60 molecules in fcc structure, which are weakly bonded via van der Waals interactions, are connected to its neighbouring molecules under high temperature and high pressure, leading to the two-dimensional layered insulating rhombohedral polymer 2D-r, which is further polymerized under higher pressure and temperature into the three-dimensional polymer 3D-r. We searched for a new rhombohedral structure of C_{60} polymer using ab initio calculations of the electronic structures and compared it with the experimentally observed data. In addition we quantitatively analyzed how the differenece between the chemical bondings in these structures affect their energetics.

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