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New hybrid materials from compressing intercalated fullerides¹ MINGGUANG YAO, BINGBING LIU, WEN CUI, JUNPING XIAO, State Key Laboratory of Superhard Materials, Jilin University — Upon compression, molecular crystal undergoes complicated transformations, including the crystal structure, molecular morphology, and inter- and intra-molecular bonding. Here, we studied a series of two-component fullerides composed of C60 molecules and various dopants under pressure and demonstrate the effect of the dopants on the structural evolution of C60s upon compression. C60 molecules are found to behave similarly, deformed and even collapsed at critical pressures, while the different interactions between the intercalated dopants and C60s result in different properties of the phases formed at high pressure. A class of new hybrid structures has been fabricated, in which several superhard phases have been discovered. The underlying mechanism for the superhard phase formation has been further uncovered.

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