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Magnetic molecules made of nitrogen or boron-doped fullerenes<sup>1</sup> CHIH-KAI YANG, Chang Gung University — By using density functional theory we investigate the electronic structure of a fullerene C60 molecule doped with nitrogen atoms. We find that as long as the number of the impurity atoms is odd the doped fullerene turns magnetic, with its magnetic moment determined by the way the impurities are bonded with the carbon cage. For even number of impurities the pairing of the electrons exclude the appearance of magnetism. Similar results also apply to fullerenes doped with boron. This simple way of creating single molecular magnets should be useful for the application in magnetic detection, quantum information, and spintronics.

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