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Oxygen Molecule Adsorption and Dissociation on Boron-doped Fullerene BC_{59} SHIZHONG YANG, LEI ZHAO, FENG GAO, GUANG-LIN ZHAO, EBRAHIM KHOSRAVI, DIOLA BAGAYOKO, Southern University and A&M College — We studied the oxygen molecule adsorption and dissociation on boron-doped fullerene (B-C_{59}) from first principles spin polarized density functional theory method simulation. The results show that O_2 molecule can be adsorbed and partially reduced on the Pauling sites of B-C_{59}. The results are compared with those of nitrogen-doped fullerene (N-C_{59}). From the comprehensive simulation results, some implications in catalyst application are given.

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