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Second harmonic generation in $N@C_{60}$ **and** $P@C_{60}$[1] MEGAN MORRIS, NICOLE PERIGO, GUOPING ZHANG, Department of Chemistry and Physics, Indiana State University, Terre Haute, IN 47809 — The successful implantation of nitrogen and phosphorus into C_{60} opens many new applications. For instance, both $N@C_{60}$ and $P@C_{60}$ are ideal candidates for quantum computing. In this paper, we show that $N@C_{60}$ and $P@C_{60}$ can be used to generate the second harmonic generation. If N and P are at the center of the buckyball, the signal is zero, but if they are off the center, the signal comes out. Therefore, the oscillation of N and P atoms will generate a 0-1-0-1 bit, when detected along the incident light direction. If this signal is sent to another $N@C_{60}$ and $P@C_{60}$, they can control the sequence of bits. The intensity sensitively depends on the laser energy and polarization. This process can be useful for quantum control by $N@C_{60}$ and $P@C_{60}$ themselves. All the results are obtained using the first-principles method.

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