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Towards *single-atom-controlled* **device**[1] SUBHASISH MANDAL, RANJIT PATI, Dept. of Physics, Michigan Technological University — *Single-atom-controlled* device has been explored recently in the context of molecular junction. Here, by using a codoping model, where a cation and an anion are introduced simultaneously into the host to maintain charge neutrality, we have probed the electron transport characteristics in a strongly coupled single molecular junction. We have used 1, 12-dicarba-*closo*-dodecaborane inorganic molecule as a precursor and have replaced one of the vertex carbon atoms by a boron atom and simultaneously decorated it with an endohedrally doped alkali atom (Li/Na) to look into the role of dopant atoms on the conductivity. The commonly used thiolate anchoring groups are used to attach the molecule in between two gold electrodes, and a parameter free, first-principles, nonequilibrium Green's function approach is used to calculate the current-voltage characteristics. Charge transfer from the alkali atom to the host is found to have a profound effect on the electronic structure causing a dramatic change in the conductivity. Since the single alkali atom controls the behavior of electron flow in this circuit, we term this device as a *single-atom-controlled* device.

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