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to determine the electron configuration for any particular atom we can build the structures in the order of atomic numbers beginning with hydrogen and continuing across the periods of the periodic table we add one proton at a time to the nucleus and one electron to the proper subshell until we have described the electron

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methods and algorithms can have far reaching impact on chemistry physics and materials

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this article provides a review of the ab initio electronic structure calculations using nao bases we begin by introducing basic formalisms of the nao based electronic structure method including nao base set generation self consistent calculations force and stress calculations

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our results for the normal state electronic structure and correlation effects in lno show much in common with the infinite layer and bilayer nickelates with remarkable site and orbital

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